The $N$-Leg spin-$S$ Heisenberg ladders: A DMRG study

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(Dated: March 18, 2014)

We investigate the $N$-leg spin-$S$ Heisenberg ladders by using the density matrix renormalization group method. We present estimates of the spin gap $\Delta_s$ and of the ground state energy per site $e_s^N$ in the thermodynamic limit for ladders with widths up to six legs and spin $S \leq \frac{1}{2}$. We also estimate the ground state energy per site $e_{2N}^L$ for the infinite two-dimensional spin-$S$ Heisenberg model. Our results support that for ladders with semi-integer spins the spin excitation is gapless for $N$ odd and gapped for $N$ even. Whereas for integer spin ladders the spin gap is nonzero, independent of the number of legs. Those results agree with the well known conjectures of Haldane and Sénéchal-Sierra for chains and ladders, respectively. We also observe edge states for ladders with $N$ odd, similar to what happens in spin chains.

PACS numbers: 75.10.Jm, 75.10.Pq

I. INTRODUCTION

The theoretical study of strongly correlated systems is undoubtedly an extremely complicated task due to the lack of appropriate techniques to address such systems, especially in dimensions greater than one. The main difficulty in the investigation of those systems is associated to the fact that the Hilbert space grows exponentially with the system size. In the last decades a great deal of effort has been devoted to develop new techniques for dealing with this issue. A major breakthrough, in this area, was the development of the density matrix renormalization group (DMRG) by White. The success of the DMRG resides in the choose of the optimal states used to represent a Hamiltonian, which are selected through the reduced density matrix eigenvalues. Usually, only a small percentage of the whole Hilbert space is necessary to describe the low energy physics of a system by using the DMRG. Due to this fact the DMRG became one of the most powerful techniques to deal with strongly correlated systems in one-dimension. Although the DMRG is based on a one-dimensional algorithm, it has been applied to low dimensional systems such as the ladder systems. The procedure consists in mapping the low-dimensional model on a 1D model with long range interactions. In this vein some other algorithms, based in the tensor networks, have been proposed to study strongly correlated systems in dimensions higher than $d = 1$, such as PEPS and MERA. Note that in dimensions $d > 1$ there are few accurate results which can be used as benchmark.

One of the goals of this work is to provide accurate results of the $N$-leg spin-$S$ Heisenberg ladders, with spin up to $S = \frac{1}{2}$, which may be used as benchmark for the new algorithms that have been proposed. Besides, and not less important, we intend to verify the Haldane-Sénéchal-Sierra conjecture, which dictates the behavior of the spin gap of the spin-$S$ Heisenberg chains and ladders.

The $N$-leg ladders are characterized by $N$ parallel chains coupled one to each others, such that the coupling $J$ along the chains is comparable to the coupling $J_\perp$ between the chains (see Fig. 1). The $N$-leg ladders are easier to deal with than the two-dimensional systems and are used as an simple route to study the last ones. In this work, we focus in legs formed by spin-$S$ Heisenberg chains. It is well known that the spin-$S$ Heisenberg model is gapped. In Ref. 26 Haldane by using a semi-classical limit of the Heisenberg chain noted that semi-integer (integer) spin Heisenberg chains are gapless (gapped), this latter statement is known as Haldane conjecture. Although the semi-classical approach is valid for $S \gg 1$ the conjecture was verified numerically for $S \geq 1/2$. In the context of the ladder systems, the same natural question arises. Dagotto et al., in Ref. 27 were the first to show that the two-leg spin-$\frac{1}{2}$ Heisenberg ladder is gapped. In Ref. 28 Rice et al. argued that spin-$1/2$ Heisenberg ladders with an odd (even) number of legs are gapless (gapped). Indeed this was verified numerically with DMRG (see also...
avoid metastable configurations we start the truncation typically $10^3$ in the final DMRG sweeps and the discarded weight was tonian above, keeping up to $3600$ states per block. In order to avoid metastable configurations we start the truncation process with large values of $m$ (typically we start with $m_{eq} \sim 1200$). In the next section we present our results for the spin-$S$ 3-leg Heisenberg ladders: estimates of the ground state energy per site ($e_N^\infty$) as well the estimates of the spin gap ($\Delta_s$) in the thermodynamic limit. We also show estimates of the ground state energy per site of the two-dimensional spin-$S$ Heisenberg model. A discussion of an edge effect, similar to what happens in the spin-1 chain, is also reported for ladders.

Before we start presenting our results, let us briefly describe the procedure we used to calculate the energies of ladder systems by using the DMRG. As we already mentioned before, the DMRG algorithm is essentially a 1D algorithm. However, it is possible to map the cluster of size $N \times L$ in a one-dimensional system with long-range interactions, as illustrated in Fig. 1. Before being reached a specific cluster size (as the one presented in Fig. 1) we need to grow the size of the system starting with four sites. In the infinite system DMRG algorithm at each step two sites are added, as illustrated in the Fig. 2 for the case of a 3-leg ladder. It is very interesting to note that, as in the one-dimensional case, we can also use the infinite system DMRG algorithm to obtain the ground state energy per site, in the thermodynamic, $e_N^\infty$ of the $N$-leg ladders. The energy per site can be estimated from the difference in energy of different iterations. Note that some energies (associated with some interactions) can not be used to estimate $e_N^\infty$, since not all steps have the correct number of sites for a fixed geometry (see Fig. 2). We estimate $e_N^\infty$ by using the following equation

$$e_N^\infty = \lim_{L \to \infty} \frac{E[N(L+2)] - E(NL)}{2N}, \quad (2)$$

where $E(M)$ is the ground state energy of a system with $M$ sites. To our knowledge this simple procedure to estimate $e_N^\infty$ for ladder systems was not used in the literature before.

II. RESULTS

The ground state energy per site: $e_N^\infty$

In Table I, we present our accurate estimates of $e_N^\infty$ for several values of $N$ and $S$. In order to get these estimates we first used Eq. (2) for a fixed number of states kept in the truncation process ($m$) and increase $L$ until the results converge (for large values of $m$ and $N$ the number of iterations is of the order of one thousand). We then get another estimate with a larger value of $m$ (typically two times larger) and we compare this estimate with the previous one. The number of digits shown in this table corresponds to the precision we get considering $m_{eq}$. The results presented in parentheses are some of the best estimates known in the literature (see also Refs. 37–42 for similar estimates). As we can see, our estimates are in perfect agreement with those results.
Table I: Estimates of the ground state energy per site $e_N^S$ for the $N$-leg spin-$S$ Heisenberg ladders. The results in parentheses are some of the best estimates known from the literature. Estimates of the ground state energy per site of the infinite two-dimensional system is also acquired by an extrapolation (see text).

| $N$ | $S = \frac{1}{2}$ | $S = 1$ | $S = \frac{3}{2}$ | $S = 2$ |
|-----|-----------------|-----------|-----------------|--------|
| 1   | -0.4431471      | -1.40148408397 | -2.828337      | -4.761248      | -7.1924 |
|     | (-0.4431471...) [Ref. 27] | (-0.14014840389) [Ref. 45] | (-0.283333) [Ref. 46] | (-4.7612481) [Ref. 47] | (-7.19223) [Ref. 48] |
| 2   | -0.578043140180 | -1.878372746  | -3.930067      | -6.73256       | -10.2852 |
|     | (-0.57802) [Ref. 27] | (-0.1878372746) | (-0.3930067) | (-0.673256) | (-1.02852) |
| 3   | -0.6005376      | -2.0204      | -4.446         | -7.669         | -11.76 |
|     | (-0.60063) [Ref. 27] | (-0.20204) | (-0.4446) | (-0.7669) | (-1.176) |
| 4   | -0.618566       | -2.0957      | -4.761248      | -8.6224       | -13.2 |
|     | (-0.61873) [Ref. 27] | (-0.20957) | (-0.4476125) | (-0.86224) | (-1.32) |
| 5   | -0.62776        | -2.141       | -5.105         | -8.865        | -12.08 |
|     | (-0.62784) [Ref. 27] | (-0.2141) | (-0.5105) | (-0.8865) | (-1.208) |
| 6   | -0.6346         | -2.169       | -5.404         | -9.469        | -12.1 |
|     | (-0.6351) [Ref. 27] | (-0.2169) | (-0.5404) | (-0.9469) | (-1.21) |
| $\infty$ | -0.66931      | -2.327       | -5.904         | -10.076       | -13.2 |
|     | (-0.66931) [Ref. 44] | (-0.2327) | (-0.5904) | (-1.0076) | (-1.32) |

Since we were able to get accurate estimates of $e_N^S$ for legs up to $N = 6$ we decide to estimate the ground state energy per site $e_2^D$ of the infinite two-dimensional system by assuming that $e_2^D (N, L = \infty) = e_N^S$ behaves as

$$e_N^S = e_2^D + \frac{A}{N}.$$  (3)

The above behavior is expected even for non-interacting systems, as shown below. Consider the following non-interacting Hamiltonian

$$H = - \sum_{<i,j>,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + H.c.),$$

where $c_{i,\sigma}$ annihilates a electron at site $j$ with spin projection $\sigma$. Here $(ij)$ denotes nearest-neighbor sites and we are considering periodic (open) boundary condition in the direction x (y). Let $L (N)$ be the number of sites in the x (y) direction. It is not difficult to shown that the ground state energy at the half-filling for $L \rightarrow \infty$ is given by

$$\lim_{L \rightarrow \infty} \frac{E(N, L)}{L} = -4 \sum_{j=1}^{N} \frac{1}{\pi} \sin \left( \frac{N-j+1}{N+1} \right) \cos \left( j\pi/(N+1) \right).$$

The leading finite-size corrections of the above equation can be obtained by using the Euler-MacLaurin formula (see for example Ref. 43 for a similar case of a two-leg spin ladder). The result obtained is

$$\lim_{L \rightarrow \infty} \frac{E(N, L)}{NL} = \frac{16}{\pi^2} + \frac{(2 - 16/\pi^2)}{N^2},$$

which presents a scaling form similar to one of Eq. (3).

In Fig. 3, we show $e_N^S$ as function of $1/N$ for several values of spins. The symbols in this figure are the numerical data and the dashed lines connect the fitted points using Eq. (3). As we can observe from the figure, the fits are very good. The values of $e_2^D$ obtained from the fits are also listed in Table I. As we can see in this table, our estimate for the case $S = 1/2 (e_2^{2D} = -0.6768)$ agrees with the one obtained by Monte Carlo method ($e_2^{2D} = -0.66931$). The origin of the very small difference (0.007) between these two values is very probably associated with the small lattice sizes considered to extrapolated our data.

The spin gap: $\Delta$.

Let $E_0(S_{\text{tot}})$ be lowest energy in the sector $S_{\text{tot}} = \sum_{i,j} < S_{i,j}^z >$. The spin gap is given by $\Delta = E_0(n) - E_0(0)$, where $n = S + 1$ if $S$ is odd and $S$ is integer (semi-integer), and $n = 1$ otherwise. By using this definition we obtain the correct spin excitation associated with the spin gap, as we explain in the following.

It is well known that the ground state of Heisenberg chains ($N = 1$) with integer spins can be understood by the valence bond solid (VBS) picture. Open spin-S chains that are described by VBS states have effective $S_{\text{end}} = S/2$ spins at each edge. Due to this fact the ground state, in the thermodynamic limit, is $(S + 1)^2$-fold degenerate. Indeed, this degeneracy has been observed in open spin-S Heisenberg chains (see for example...
Ref. 51). Due to this fact, the mass gap for the integer spin-$S$ chains, under open boundary condition, must be calculated from the singlet ground state to the lowest excited state in the sector $S_{\text{tot}} = S + 1$ [or equivalently, $E_0(S + 1) - E_0(S)$]. This degeneracy can be understood by the edge spins that in the thermodynamic limit do not interact with each others.50

By analyzing the topological term of the non-linear sigma model $N_g$ in Ref. 51 proposed that spin-$S$ chains with semi-integer spins also present edge spins of magnitude $S_{\text{end}} = (S - 1/2)/2$. Theses edge spins indeed have been observed.48,52,53 Due to this fact, the spin gap excitation of chains with semi-integer spin that must be investigated is $\Delta = E_0(S + 1/2) - E_0(0)$.

The most beautiful signature of the edge states appears in the measured value of $S_{1,j}$ in the sector $S_{\text{tot}} = S$ $[S - 1/2]$ for integer [semi-integer] spins. Let us focus, first, in the results of integer spins. We show in Figs. 4(a) the local values of $S_{1,j}$ for chains with $S = 1, 2$ and $S = 3$ (similar results can be found in Refs. 52 and 53 for $S = 1$ and 2). It is clear from this figure, that a $S_{\text{end}} \equiv S/2$ spin appears at the end of the spin-$S$ chains. We found $S_{\text{end}} = 0.53, 1.12$, and $1.64$ for the chains with $S = 1, 2$ and 3, respectively. As we can see from this figure, the log-linear plot shows an exponential decay. The decay lengths $\xi^S$ obtained by the slope of straight lines are: $\xi^1 = 5.94$ and $\xi^2 = 47.5$. The decay length $\xi^1$ is very close to the one found by White in Ref. 5 (\(\xi^1 = 6.03\)). On the other hand, our result for $\xi^2$ differ from two previous estimates ($\xi^2 = 49.1$ and $\xi^2 = 54.3$, see Refs. 47 and 11). It is also very interesting to notice that in order to see the exponential decay of $S_{1,j}$ from the edge, the size of the systems can not be smaller than the decay length $\xi^S$ [see inset of Fig. 4(a)].

Our result for the case $S = 3$ [inset of Fig. 4(a)] shows that even considering a chain of size $L = 800$ we were not able to see yet an exponential decay. For chains with semi-integer spins our results support that $S_{\text{end}} = (S - 1/2)/2$, as expected.48,52,53 We found that $S_{\text{end}} = 0.57$ and 0.94 for chains with spin $S=3/2$ and $S=5/2$, respectively. In

Figure 3: (color online) Ground state energy per site of infinite N-leg Heisenberg ladders $\varepsilon^S_{\text{tot}}/S^2$ vs $1/N$ for spins up to $S=3/2$ (see legend). The dashed lines are fits to our data using Eq. 9 (see text).

Figure 4: (color online) (a) A log-linear plot of $2 |<S_{1,j}^t>|/S$ for chains with $L = 400$ and $S = 1$ and 2. Inset: a linear-linear plot for three values of $S$. (b) $2N |<S_{1,j}^t>|/S$ vs $j$ for some ladders of size $L = 60$ with spins 1 and 2 (see legend). (c) $2N |<S_{1,j}^t>|/(S - 1/2)$ vs $j$ for ladders with spins 3/2 and 5/2. Only few sites are presented. (d) Values of $<S_{1,j}^t>$ measured in the two first rungs of ladders with integer spins. The size of the arrows indicates the magnitude of $<S_{1,j}^t>$. The scale used is also presented.
those latter cases, we found that $< S_{i,j}^z >$ exhibits a power-law decay [see Fig. 4(c)], as expected for open critical systems.

A similar effect that resembles what happens in chains also appears for ladders only if $N$ is odd, as depicted in Figs. 4(b) and (c) for integer and semi-integer spins, respectively. However, in this latter case the end spin $S_{end} = \sum_{j=1}^{[N/2]} < S_{1,j-1}^z >$ (where $[N/2]$ is the largest integer less than or equal to $N$): (i) is spread along the end rung [see Fig. 4(d)] and (ii) the value of $S_{end}$ decreases with the increasing of $N$. For example for $S = 1$, we found that $S_{end} = 0.45, 0.33, 0.22$ and $0.19$ for $N = 3, 5, 7$ and 9, respectively. For $N$ even our results show the absence of this edge effect, as shown in Figs. 4(b) and 4(c).

We can use a heuristic argument to understand the fact that the edge states of ladders appear only for $N$ odd. Consider the strong coupling limit, i.e., the coupling along the rung is much larger than the coupling along the chains. If the number of legs is even (odd) the ground state of the rung is a singlet (S-plet). So, “rung sites” behave as an effective spin-$S$ if $N$ is odd. For this reason, we may expect that $S_{end} = 0$ for $N$ even and $S_{end} = S/2$ for integer [semi-integer] spins and $N$ odd. Indeed, our results presented in Figs. 4(a)-(c) support this picture [see also Figs. 6(a)-(c)].

Finally, let us show our results for the spin gap. In Figs. 5(a)-(d), we present the finite-size spin gap $\Delta(L)$ as a function of $1/L$ for ladders with $S = 1/2, 3/2, 5/2$ and 1 and some values of $N$. In order to estimate the spin gap in the thermodynamic limit ($\Delta_s$) we assume that $\Delta(L)$ behaves as

$$\Delta(L) = \Delta_s + \frac{A}{L} + \frac{B}{L^2}$$  \hspace{1cm} (4)$$

It is expected that the spin gap of open chains with integer spins behaves as $\Delta(L) \geq \Delta_s + a_1/L + a_2/L^2$, as expected for open critical systems. Indeed, previous studies of the spin-1 chain found that $\Delta(L)$ scale with $1/L^2$ for large values of $L$. We also have observed this behavior for the spin-1 chain [see Fig. 5(d)]. We have added the $1/L$ term because our results show that the leading finite-size correction of $\Delta(L)$ is $1/L$ for small system sizes. Note that if we consider the energy dispersion $\Delta(k) = \sqrt{\Delta_m + (vk)^2}$ for a magnon with wave vector $k$, as pointed out by S. Qin et al. in Ref. 55, we see that $\Delta \sim \Delta_m + (2k^2)/2\Delta_m$ only if $L \gg \Delta_m$. This suggests that leading finite-size correction of $\Delta(L)$ is $1/L$ when the lattice sizes are smaller than the correlation length. Even though the asymptotic scaling form is not reached, it is possible to obtain reasonable estimates of $\Delta_s$ by using Eq. (4), as we explain in the following. It is possible to fit our data by using only the $1/L$ ($1/L^2$) term in order to obtain a lower (upper) bound and then quote an estimative of the spin gap by an average of these two values, as done by Schollwöck and Jolicoeur in Ref. 17. We notice that if we fit our data with the two terms, simultaneously, we get estimates very close to the procedure used by Schollwöck and Jolicoeur, i.e., an estimate between the upper and lower bound. For example, for the spin-2 chain we got $\Delta_s = 0.084$ by considering $200 < L < 400$ (it is interesting to mention that it was found $\Delta_s = 0.07 \pm 0.02$ in experimental realization of the spin-2 chain55). If we had considered systems with sizes $20 < L < 120$ to extract the spin gap, we would find $\Delta_s = 0.04$. This shows that if we consider system sizes smaller than the correlation length to determine $\Delta_s$. The estimate obtained should be interpreted as a lower bound estimate. Finally, we should mention that in principle logarithmic corrections like $1/L \ln L$ are also expected due to the marginally irrelevant operators. However, we notice that if we replace the last term of Eq. (4) by the logarithmic correction term $1/L \ln L$, the fits obtained are slightly worse than the ones found using the Eq. (4).

As we already mentioned, it is expected that the $N$-leg spin-$S$ Heisenberg ladders is gapless (gapped) if $SN$ is semi-integer (integer). Indeed, as we can observe in Figs. 5(a)-(d) our results, overall, are consistent with the Haldane-Sénéchal-Sierra conjecture. We found that for ladders with $SN$ semi-integer that the extrapolated values of $\Delta_s$ are $\approx 10^{-3}$. These latter results strongly indicate that the spin gap is zero for ladders with $SN$ semi-integer. In order to better visualize the results of $\Delta_s$, we report in Table III the extrapolated values we got from the fit procedure. In this table, we also present some estimates of $\Delta_s$ found in the literature. As we can see, our results are similar to those found in the literature and, within our precision, our results agree perfectly with the Haldane-Sénéchal-Sierra conjecture. Note that the spin gap decreases with the number of legs and the values of $L$. For example, for the spin-$2$ chain we got $\Delta_s = 0.084$ by considering $200 < L < 400$ (it is interesting to mention that it was found $\Delta_s = 0.07 \pm 0.02$ in experimental realization of the spin-2 chain55). If we had considered systems with sizes $20 < L < 120$ to extract the spin gap, we would find $\Delta_s = 0.04$. This shows that if we consider system sizes smaller than the correlation length to determine $\Delta_s$. The estimate obtained should be interpreted as a lower bound estimate. Finally, we should mention that in principle logarithmic corrections like $1/L \ln L$ are also expected due to the marginally irrelevant operators. However, we notice that if we replace the last term of Eq. (4) by the logarithmic correction term $1/L \ln L$, the fits obtained are slightly worse than the ones found using the Eq. (4).
Table II: Estimates of the spin gap $\Delta_s$ for the Heisenberg ladders with up to six legs and $S \leq \frac{7}{2}$. These values were extracted from the fit of our data using the equation (4). The results in parentheses are some of the best estimates known from the literature.

| $N$ | $S = \frac{1}{2}$ | $S = 1$ | $S = \frac{3}{2}$ | $S = 2$ | $S = \frac{5}{2}$ |
|-----|-----------------|---------|-----------------|---------|----------------|
| 1   | --              | 0.41025 | --              | 0.084   | --              |
|     | (0.41050) [Ref. 45] | --       | (0.085) [Ref. 47] | --       | --              |
| 2   | 0.5011          | 0.151   | 0.036           | 0.013   | 0.01           |
|     | (0.504) [Ref. 4] | --       | --              | --       | --              |
| 3   | --              | 0.017   | --              | 0.01    | --              |
| 4   | 0.15            | 0.015   | 0.007           | --      | --              |
|     | (0.17) [Ref. 27] | --       | --              | --       | --              |
| 5   | --              | --      | --              | --      | --              |
| 6   | 0.05            | (0.05) [Ref. 27] | --       | --      | --              |

Figure 6: (color online) (a), (b) and (c): the spin excitation $\Delta E(S_{tot}^z)$ as function of $1/L$ for the 3-leg Heisenberg ladders for $S = 1$, $S = 2$, and $S = 3/2$ and some values of $S_{tot}^z$ (see legend). The symbols are the numerical data and the lines in these figures connect the fitted points (see text). Insets: zoom of the region close to zero.

As we discussed earlier, due to the edge states we expect that the ground state is $(S + 1)^2$-fold degenerate, in the thermodynamic limit, for ladders with integer [semi-integer] spins if $N$ is odd.

In order to verify this claim, we also calculate the spin excitations $\Delta E(S_{tot}^z) = E_0(S_{tot}^z) - E_0(0)$, for few values of $S_{tot}^z$. In Figs. 6(a)-(c), we show the spin excitation $\Delta E(S_{tot}^z)$ for 3-leg ladders with spins $S = 1$, 2 and 3/2. The results for the 3-leg spin-1 Heisenberg ladder, presented in Fig. 6(a), in fact indicate that $E_0(1) = E_0(0)$ in the thermodynamic limit, as we expect. For larger values of $S$, as we illustrate in Fig. 6(b)-6(c) for the cases $S = 2$ and $S = 3/2$, it is very difficult to see accurately if the ground state is degenerate (due mainly to the system sizes we consider). Nevertheless, our results within of the accuracy of the extrapolations are consistent with the fact that the ground state is $(S + 1)^2$-fold degenerate, for ladders with integer [semi-integer] spins and $N$ odd. Besides that, if we had estimated the spin gap for ladders with integer spins considering only $\Delta E(1)$, we would find that the spin gap for $N = 4$ would be larger than $N = 3$, which is not expected. For these reasons we do believe that the ground state is degenerate, in the thermodynamic limit, for ladders with $N$ odd.

III. CONCLUSIONS

In this work, we use the unbiased DMRG method to investigate the $N$-leg spin-$S$ Heisenberg ladders. While the low energy physics of the Heisenberg chains and the spin-1/2 Heisenberg ladders were studied by several works, few is known about the Heisenberg ladders with spin $S \geq 1$. We made a great numerical effort to provide some precise estimates of the ground state energy per site $e_N^\infty$ in the thermodynamic limit for the Heisenberg ladders. We also present several new estimates of the spin gap $\Delta_s$, which were unknown, mainly for $N > 1$ and $S \geq 1$. Our estimates for spin-$S$ chains and for spin-1/2 ladders are similar to those known in the literature. Our results corroborate with the Haldane and Sénéchal-Sierra conjectures for chains and ladders, which establish that the $N$-leg spin-$S$ Heisenberg ladders is gapless (gapped) if $SN^2 \exp(-SNa)$, where $a$ is constant.
is semi-integer (integer). We also observe edge states for ladders if $N$ is odd that resemble the edge states found in chains. We believe that this latter result will help understanding more deeply the nature of the ground state of the Heisenberg ladders.

Acknowledgments

The authors thank G. Sierra and J. A. Hoyos for useful discussions. This research was supported by the Brazilian agencies FAPEMIG and CNPq.

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