We study numerically the dimerized Heisenberg model with frustration appropriate for the quasi-1D spin-Peierls compound CuGeO$_3$. We present evidence for a bound state in the dynamical structure factor for any finite dimerization $\delta$ and estimate the respective spectral weight. For the homogeneous case ($\delta = 0$) we show that the spin-wave velocity $v_s$ is renormalized by the n.n.n. frustration term $\alpha$ as $v_s = \pi/2J(1-b\alpha)$ with $b \approx 1.12$

Quantum 1D spin systems may show a variety of instabilities. Of particular interest is the spin-Peierls (SP) phase due to residual magnetoelastic couplings \cite{1}, which leads to the opening of a gap in the spin excitation spectrum. The discovery \cite{2} of the spin-Peierls transition below $T_{SP} = 14$ K in an inorganic compound, CuGeO$_3$, has attracted widespread attention.

The spin-dynamics of CuGeO$_3$ is being studied intensively \cite{3,4}. Above the spin-Peierls transition, the one-magnon excitation spectrum, as measured by neutron scattering \cite{5}, forms a broad continuum. The form of the continuum is in good agreement with the continuum expected for one-dimensional antiferromagnetic Heisenberg chains \cite{6}; it is also seen in the magnetic Raman spectrum \cite{7}. The physics behind the continuum in the one-magnon excitation spectrum lies on the fact that the elementary excitations of the one-dimensional Heisenberg chain are spinons (also called solitons or Bloch walls), each magnon being made up of two solitons. The resulting “two-spinon” continuum has been seen experimentally also in other quasi-1D antiferromagnets \cite{8}.

The exact form of the magnetic excitation spectrum in the dimerized state below $T_{SP}$ is still being investigated. A two-spinon continuum is observed \cite{9,10} with large spectral weight at the lower edge. The dispersion of the lower edge has been used to extract the spin-wave velocity \cite{10}. Muthukumar et al. have pointed out recently \cite{11} that the experimental magnetic Raman intensity indicates a well defined magnon mode in the spin-Peierls state of CuGeO$_3$ and that the origin of this magnon could not be determined on the basis of the Raman scattering data obtained numerically for a single chain.

The existence of a well defined magnon mode, i.e. a two-spinon bound state which splits of the continuum, has also been addressed recently by Uhrig and Schulz \cite{12} within an RPA approach. A recent neutron scattering experiment \cite{13}, has been interpreted as indicative of such a bound-state.

In this context it is an important question to address whether other techniques can shed light on the magnetic excitation spectrum of the dimerized Heisenberg model. Here we present data for the dynamical structure factor $S(k, \omega)$ obtained by applying the recursion method \cite{14} to calculate the excitation spectrum of the hamiltonian given below. This approximate method in particular gives very accurate results for the low-lying excitations. We find evidence for a bound-state for any dimerization $\delta > 0$, independently of the amount of frustration $\alpha$ present. The finite-size corrections of the data is, for certain $k$-values, small enough to determine accurately the position of the bound state and its spectral weight. We furthermore determine the renormalization of the spin-wave velocity in the homogeneous state as a function of the frustration. The magnetic properties of CuGeO$_3$ can be modeled by the 1D spin-Hamiltonian

$$H = J \sum_i [(1 + \delta(-1)^i) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2}]$$

where $\delta$ is the dimerization parameter that vanishes above $T_{SP}$, its zero temperature value has been estimated to be $\delta = 0.03$ \cite{15}. The exchange integral $J > 0$ and the amplitude for the frustrating n.n.n. coupling $\alpha$ have been estimated to be $J \approx 150$K \cite{15} and $\alpha \approx 0.24 - 0.36$ \cite{15,16}, respectively.

The phase diagram of $H$ in Eq. (1) has been calculated using the density-matrix renormalization-group method \cite{17}. For $\delta = 0$ and $\alpha < \alpha_c \approx 0.2411$, the ground state is gapless and renormalizes to the Heisenberg fixed point. The rest of the phase space is gapped. For $\delta + 2\alpha = 1$ the exact ground state is known to be a valence-bond state.

The dynamical structure factor $S(k, \omega)$ in the groundstate $|0\rangle$ of (1) is given by

$$S(k, \omega) = \sum_n |\langle 0 | \mathbf{S}^z(-k) | n, k \rangle|^2 \delta(\omega - (E_n(k) - E_0))$$

where $|n, k\rangle$ and $E_n(k)$ are the respective eigenstates and the eigenvalues of (1) in the subspace with total momentum $k$, $|0\rangle$ being the overall ground-state and $E_0$ the
ground-state energy. The allowed values for the momentum \( k \) are \( k = 0, 2\pi/N, \ldots, \pi \), for a finite chain of length \( N \) with periodic boundary conditions. \( S^z(k) \) is given by

\[
S^z(k) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \exp(ikx) S_x^z.
\]

We have evaluated \( S(k, \omega) \) for chains with \( N = 12, 16, 20, 24 \) using an approximate scheme for the determination of the lowest-lying excitation energies \( E_n(k, N) - E_0(N) \) and the corresponding transition probabilities \( |\langle n | S^z(k) | 0 \rangle|^2 \). Using a recursion algorithm a set of orthogonal states is built starting with \( S^z(0) \). Coefficients occurring in this procedure form a tridiagonal matrix whose eigenvalues and eigenstates determine the excitation energies and transition probabilities. (For further details and technical limitations of this method see ref. [13].)

The dynamical structure factor is given, for any finite chain, by a sum over discrete poles. The weight of the individual poles,

\[
w_n(k) = |\langle 0 | S^z(-k) | n, k \rangle|^2
\]

will go to zero in the thermodynamic limit, \( N \to \infty \), whenever the respective pole contributes to the continuum. The sum-rule

\[
\sum_n w_n(k) = S(k)
\]

(3)
is here valid, where \( S(k) \) is the static structure factor,

\[
S(k) = \langle 0 | S^z(-k) S^z(k) | 0 \rangle.
\]

(4)

We are here interested in particular in the lowest pole, located at \( E(k) = E_0(k) - E_0 \), where \( |n = 0, k\rangle \) is the lowest state with energy \( E_0(k) \) in the subspace of total momentum \( k \). We want to examine the question whether this pole is part of the continuum in the thermodynamic limit, or whether it evolves into a bound state, characterized by

\[
w_0(k) \to \text{const., } N \to \infty.
\]

(5)

In Fig. (3) we present for \( \alpha = 0 \) the relative weight of the lowest pole contributing to \( S(k, \omega) \),

\[
w_0^{(rel)}(k) = w_0(k) / S(k).
\]

(6)

The data for \( w_0^{(rel)}(k) \) presented in Fig. (3) shows a monotonic decrease for \( \delta = 0 \) as a function of chain length \( N \), indicating that the lowest pole will be part of the two-spinon continuum in the thermodynamic limit. This behaviour is what we expect for the homogeneous Heisenberg chain. For the dimerized Heisenberg chain, \( \delta = 0.1 \) in Fig. (3), we observe on the other hand for all \( k < \pi \) a monotonic increase of \( w_0^{(rel)}(k) \) with increasing chain length! This behaviour is also obtained when we introduce a finite amount of frustration \( \alpha = 0.24 \) into the system, as can be seen in Fig. (3), where we compare the data for \( \delta = 0 \) and \( \delta = 0.03 \), as appropriate for CuGeO3.

We also observe in Fig. (1) and Fig. (2) that the finite-size dependence of the relative weight of the lowest pole is small enough in the dimerized state for \( k < \pi/2 \), that an estimate of the spectral weight in the thermodynamic limit is possible for \( k \leq \pi/2 \). Taken together we conclude that the data presented in Fig. (1) and Fig. (2) clearly indicate for \( \delta > 0 \) a finite value for \( w_0(k) \) in the thermodynamic limit and therefore a bound state.

Another interesting feature of the data presented in Fig. (1) and Fig. (2) is the large dependence of \( w_0^{(rel)}(k) \) on the dimerization parameter \( \delta \). This observation is reminiscent to the large \( \delta \)-dependence observed for the Raman spectral weight in a previous study [9]. It is interesting to note that this behaviour is solely due to the \( \delta \)-dependence of the matrix element \( w_0(k) \) and that the static structure factor \( S(k) \), entering Eq. (3), is relatively size and \( \delta \)-independent for most \( k < \pi \), as can be seen from the data presented in Fig. (3).

In Fig. (3) we present for \( \alpha = 0.24 \) the data for static structure factor \( S(k) \) and the energy dispersion \( E(k) = E_0(k) - E_0 \) for both \( \delta = 0 \) and \( \delta = 0.03 \) and for \( N = 20 \) (open symbols) and \( N = 24 \) (filled symbols). We notice that the finite size effects are, in general, much smaller than those for the weight of the lowest pole presented in the previous figures and that the finite size effects for \( \delta = 0.03 \) are smaller than those for \( \delta = 0 \).

A relative large difference for \( \delta = 0 \) and \( \delta = 0.03 \) occurs, for the data presented in Fig. (3) for the “magnon dispersion” \( E(k) \), for \( k > \pi/2 \). This behaviour is a consequence of the coupling of the momenta \( k \) and \( k + \pi \) by the dimerization. For any finite \( \delta > 0 \) we have therefore the symmetry \( E(\pi/2 + \Delta k) = E(\pi/2 - \Delta k) \). In the homogeneous case, \( \delta = 0 \), one has instead that \( E(\pi/2 + \Delta k) > E(\pi/2 - \Delta k) \) for any finite chain and \( \pi/2 > \Delta k > 0 \).

In Fig. (3) we present a study of the spin-wave velocity, \( v_s \), as a function of frustration \( \alpha \) and a range of system sizes \( N = 12, 16, 20, 24 \), and \( \delta = 0 \). Here we estimated \( v_s \) using the formula

\[
v_s = \frac{E(k)}{k} \bigg|_{k = 2\pi/N}.
\]

Strictly speaking we expect \( v_s \) to diverge like \( \sim \Delta N/2\pi \) in the thermodynamic limit for any \( \alpha > \alpha_c \approx 0.2411 \) where a gap \( \Delta \) opens in the spin-wave spectrum. This divergence will be very difficult to observe in finite-size studies as the gap is exponentially small for \( \alpha \) larger but close to \( \alpha_c \).

The size-dependence of \( v_s \) is evident also for small values of \( \alpha \). For \( \alpha = 0 \) the exact values for the spin-wave velocity is known to be \( \pi/2J \) in the thermodynamic, given
by the intersect of the solid line in Fig. (4) with the y-axis. The finite size corrections do, on the other hand, actual increase slightly with increasing chain length \( N \), at least for \( N \leq 24 \) and \( \alpha = 0 \). We have therefore decided to try for a linear fit of \( v_s \) as a function of \( \alpha \) by demanding the fit to reproduce the Bethe-Ansatz value for \( \alpha = 0 \). The corresponding fit (solid line in Fig. (4)) is

\[
v_s = \frac{\pi}{2} J (1 - b \alpha),
\]

with \( b \approx 1.12 \) [19].

In conclusion we have presented numerical evidence for the occurrence of a discrete-pole contribution to the dynamical structure factor for dimerized Heisenberg chains. This contribution to \( S(k, \omega) \) may also be interpreted, at least in part, as a two-spinon bound state [11], it constitutes a well-defined magnon mode. It is interesting to note that such a bound-state would imply a peak in the two-magnon density of states and might therefore show up in the Raman-spectral weight. A previous numerical study has not found such a peak structure in the Raman spectral weight of dimerized Heisenberg chains. This discrepancy may be either due to strong magnon-magnon interaction effects in 1D spin chains or due to matrix-element effects [18].

We have furthermore presented data for the dispersion of the magnon-mode and the static structure factor, showing that the finite-size effects are small for these quantities. In addition we have estimated the renormalization of the spin-wave velocity for frustrated Heisenberg chains in the gapless region.

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FIG. 1. The relative weight \( w^{(\text{rel})}_0(k) \) of the lowest pole contributing to the dynamical structure factor \( S(k, \omega) \) for \( \alpha = 0, \delta = 0 \) and \( \delta = 0.1 \) and for chains with \( N = 16, 20, 24 \) sites respectively. The relative weight is given by \( w^{(\text{rel})}_0(k) = w_0(k)/\sum_n w_n(k) \), where the \( w_n(k) \) are the absolute weights of the poles contributing to \( S(k, \omega) \). The lines are guides to the eye.

FIG. 2. The relative weight \( w^{(\text{rel})}_0(k) \) of the lowest pole contributing to the dynamical structure factor for \( \alpha = 0.24, \delta = 0 \) and \( \delta = 0.1 \) and for chains with \( N = 16, 20, 24 \) sites respectively. The lines are guides to the eye.

FIG. 3. The energy of the lowest excited state with momentum \( k \), \( E(k) \), and the static structure factor, \( S(k) \), for \( \alpha = 0.24 \) and both \( \delta = 0 \) and \( \delta = 0.03 \). The open/filled symbols are the data for chains with \( N = 20 \) and \( N = 24 \) sites respectively. The lines are guides to the eye.

FIG. 4. The spin-wave velocity, \( v_s \), as a function of \( \alpha \) calculated for \( \delta = 0 \) and chains with length \( N = 12, 16, 20, 24 \). \( v_s \) has been determined using the formula \( v_s = (E(2\pi/N) - E(0))/(2\pi/N) \), where \( E(k) \) is the ground-state energy for chains with total momentum \( k \). The dashed lines are guides to the eye, the full line is a fit.
$\frac{k}{\pi}$

Relative weight of lowest pole

$N = 16$

$N = 20$

$N = 24$

$\alpha = 0$

$\delta = 0$

$\delta = 0.1$
The graph shows the relative weight of the lowest pole as a function of \( k / \pi \) for different values of \( \delta \) and \( N \).

- For \( \alpha = 0.24 \), the lines are labeled as follows:
  - \( \delta = 0 \) (solid line)
  - \( \delta = 0.03 \) (dashed line)

The graphs are represented with different markers and line styles for each value of \( N \):
- \( N = 16 \) (filled circles)
- \( N = 20 \) (open circles)
- \( N = 24 \) (filled squares)
$E(k)$ and $S(k)$

$\alpha = 0.24$

$\begin{align*}
N=24, \delta=0 \\
n=20, \delta=0 \\
n=24, \delta=0.03 \\
n=20, \delta=0.03
\end{align*}$
\[ \frac{v_s}{(J^\pi)} = (1-1.12\alpha)/2 \]