The susceptibility and excitation spectrum of (VO)$_2$P$_2$O$_7$ in ladder and dimer chain models

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Abstract

We present numerical results for the magnetic susceptibility of a Heisenberg antiferromagnetic spin ladder, as a function of temperature and the spin-spin interaction strengths $J_\perp$ and $J_{||}$. These are contrasted with new bulk limit results for the dimer chain. A fit to the experimental susceptibility of the candidate spin-ladder compound vanadyl pyrophosphate, (VO)$_2$P$_2$O$_7$, gives the parameters $J_\perp = 7.82$ meV and $J_{||} = 7.76$ meV. With these values we predict a singlet-triplet energy gap of $E_{\text{gap}} = 3.9$ meV, and give a numerical estimate of the ladder triplet dispersion relation $\omega(k)$. In contrast, a fit to the dimer chain model leads to $J_1 = 11.11$ meV and $J_2 = 8.02$ meV, which predicts a gap of $E_{\text{gap}} = 4.9$ meV.

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I. Introduction

Quantum antiferromagnetism in lower-dimensional systems has proven to be a very rich subject. Some of the more dramatic developments include the realization that half-integral and integral spin chains have very different excitation spectra, \[1\] and evidence that two-dimensional antiferromagnetism is a crucial component of high temperature superconductivity. \[2–4\]

The Heisenberg spin ladder is interesting theoretically as an intermediary between half-integer (\(S = 1/2\)) and integer (\(S = 0, 1\)) spin chains. This system has isotropic nearest-neighbor interactions along the chains (\(J||\)) and along the rungs (\(J\perp\)) of a ladder geometry,

\[
H = J|| \sum \leftrightarrow S_i \cdot S_j + J\perp \sum \uparrow \downarrow S_i \cdot S_j .
\]

Previous studies of the Heisenberg spin ladder have discussed the ground state energy and the dependence of the singlet-triplet energy gap on \(J\perp/J|| \equiv \alpha\ell\) in the antiferromagnetic regime, \[3,4\] the triplet spin-wave dispersion relation, \[5\] the behavior of the system under doping \[5,7\] and the dynamical structure function. \[6\] Ferromagnetic rung couplings (\(J\perp < 0, J|| > 0\)) have been studied using Lanczos and Monte Carlo techniques and the renormalization group; \[6\] these references suggest that a gap exists for all \(J\perp < 0\).

In Ref. \[7\] we presented numerical and analytical results for the ground state energy and triplet spin-wave dispersion relation of an \(S = 1/2\) spin ladder, as well as numerical results for the structure function \(S(\vec{k}, \omega)\). We found evidence that a singlet-triplet energy gap appears for any interchain coupling \(J\perp/J|| > 0\), and that the spin-wave band minimum is at \(k = \pi\), but the band is folded so the maximum energy occurs between \(k = \pi/2\) (for \(J\perp/J|| = 0\)) and \(k = 0\) (for \(J\perp/J|| = \infty\)). The bandwidth was found to be relatively insensitive to the rung coupling \(J\perp\), and varied between \(\pi J||/2\) (for \(J\perp/J|| = 0\)) and \(2J||\) (for \(J\perp/J|| = \infty\)).

The antiferromagnetic spin ladder may be realized in nature by the antiferromagnet vanadyl pyrophosphate, \[8,9\] \((VO)_2P_2O_7\). This material has a ladder configuration of \(S = 1/2\) \(V^{+4}\) ions (Fig. 2 of Ref. \[8\]), with spacings of 3.19(1) Å between rung ions and 3.864(2) Å between rung ions.
Å between chain ions, and has a magnetic susceptibility characteristic of an antiferromagnet with an energy scale (from the susceptibility maximum) of \( \approx 7 \text{ meV} \). The closely related material \( \text{VO(HPO}_4\cdot{\frac{1}{2}}\text{H}_2\text{O} \) has isolated \( V^{+4} \) ion pairs at a similar separation of 3.10 Å, and is well described magnetically by independent spin-1/2 Heisenberg pairs with a coupling (in our conventions) of \( J = 7.81 \text{ meV} \). [10]

Although the \( \text{(VO)}_2\text{P}_2\text{O}_7 \) lattice clearly shows a ladder configuration of \( V^{+4} \) ions, they might in principle interact magnetically as a different spin system. This was the case for \( \text{Cu(NO}_3\cdot{5}\text{H}_2\text{O} \) (Ref. [11]), which was originally considered to be a possible spin ladder system but was subsequently found to interact as a dimer chain, described by the Hamiltonian

\[
H = \sum_i \left\{ J_1 \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} + J_2 \mathbf{S}_{2i+1} \cdot \mathbf{S}_{2i+2} \right\},
\]

with \( J_2/J_1 \equiv \alpha_d \) (\( 0 \leq \alpha_d \leq 1 \)). It was not practical to distinguish between ladder and dimer chain models of copper nitrate from bulk thermodynamic properties alone, which were found to be very similar for the two systems. [11] The issue was finally decided in favor of the dimer chain model by proton resonance [12] and neutron diffraction [13] experiments.

Vanadyl phosphate presents similar ambiguities. Although its susceptibility has been measured and is accurately described by the susceptibility of a dimer chain [9] (2), it is widely believed that the ladder Hamiltonian (1) will lead to a very similar \( \chi(T) \) and so is not excluded by the good agreement with the dimer chain. Since no theoretical results have been published for the bulk limit ladder susceptibility in the relevant \( J_\perp \sim J_\parallel \) regime, comparison of the experimental susceptibility to the ladder model has not been possible. In this paper we present new numerical results for the bulk limit susceptibility of ladders and dimer chains, and fit these to the data for \( \text{(VO)}_2\text{P}_2\text{O}_7 \). As we shall see, these two models do give very similar results for the susceptibility, and both give excellent fits to \( \text{(VO)}_2\text{P}_2\text{O}_7 \) with appropriate parameters. The ladder \( \chi(T) \) is preferred, although the differences may be less important than the approximations made in the models.
II. Spin ladder and dimer chain susceptibilities

We determined the susceptibility on finite lattices by generating all energy levels \( \{E_i\} \) and their multiplicities \( \{d_i\} \) in each sector of fixed total \( S_z \), using a Householder algorithm. The susceptibility was then obtained through its relation to the expected squared magnetization, summed over energy levels and total \( S_z \) sectors;

\[
\chi(T) = g^2 \langle \mu_B \rangle^2 \frac{\sum_S S_z \sum_i S_z^2 d_i e^{-\beta E_i}}{\sum_S \sum_i d_i e^{-\beta E_i}}.
\]

This approach has the advantage that explicit eigenvectors are not required. For the ladder geometry we used (3) to determine \( \chi \) on \( 2 \times L \) lattices with \( L = 3, 4, \ldots, 8 \) for couplings \( J_\perp/J_{||} = \alpha_\ell = 0.5, 0.7, 0.9, 1.0 \) and 1.1 and for a range of \( T/J_{||} \) values; for reference purposes the \( 2 \times 8 \) results are given in Table I. To estimate the bulk limit susceptibility the \( 2 \times L \) results were fitted to the form \( \chi_L = \chi_\infty + ae^{-bL} \) at each \( T \) and coupling, independently for \( L = \text{even} \) and \( L = \text{odd} \), since these approached the bulk limit from opposite directions. This gave independent estimates of the bulk limit susceptibility, which allowed a test of the accuracy of our extrapolation in \( L \). Our bulk limit estimate was taken to be the average of the even-\( L \) and odd-\( L \) extrapolated values. For the dimer chain we followed a similar procedure for parameter values \( J_2/J_1 = \alpha_d = 0.2, 0.4, \ldots, 1.0 \) and \( L = 4, 6, \ldots, 16 \); Table II gives the \( L = 16 \) results. For the dimer chain there is no odd/even effect in the long axis (we always assume an even number of spins so the ground state has no net magnetization), so we had only a single extrapolation in \( L \) for each \( T \). This was compensated by smaller finite size artifacts than on the ladder, because the long axis of the dimer chain spanned a maximum of 16 rather than 8 spins. For fitting purposes it is useful to have a parametrization of these results that allows accurate interpolation in \( T \) and interaction strengths. We tested several forms and found that the six-parameter function

\[
\chi(T) = \frac{c_1}{T} \left[ 1 + \left( \frac{T}{c_2} \right)^{c_3} \left( e^{c_4/T} - 1 \right) \right]^{-1} \left[ 1 + \left( \frac{c_5}{T} \right)^{c_6} \right]^{-1}
\]

adequately describes both the experimental data \([14]\) and the theoretical ladder and dimer chain susceptibilities over a range of parameters relevant to \((\text{VO})_2\text{P}_2\text{O}_7\). This form also has
the advantage that it incorporates the exponential behavior expected at low temperatures, unlike other parametrizations used previously for the dimer chain, and at high temperature it gives the correct Curie form $g^2\mu_B^2/4k_BT$. (The overall normalization $c_1$ is identically equal to $g^2\mu_B^2/4k_B$ in all cases, but the $V^{4+}$ ion $g$-factor is unknown \textit{a priori} and is determined when $c_1$ is fitted to the data.)

For the two theoretical susceptibilities we fitted our numerical bulk limit results to (4), with each of the coefficients $c_2, \ldots, c_6$ taken to be quadratic in the ratio of the two coupling constants. Preliminary fits to the (VO)$_2$P$_2$O$_7$ susceptibility indicated that the values $\alpha_\ell = 1.0$ and $\alpha_d = 0.7$ were close to optimum, so we parametrized our bulk limit results in terms of the departure from these values. The fitted coefficients $c_2 \ldots c_6$ for the ladder over the range $0.9 \lesssim \alpha_\ell \lesssim 1.1$ (with $J_{||} = 1$) were found to be

$$c_2 = +2.315 - 4.035(\alpha_\ell - 1.0) + 7.050(\alpha_\ell - 1.0)^2$$  \hspace{1cm} (5a)
$$c_3 = +0.403 - 1.025(\alpha_\ell - 1.0) + 1.850(\alpha_\ell - 1.0)^2$$  \hspace{1cm} (5b)
$$c_4 = +0.443 + 0.225(\alpha_\ell - 1.0) + 0.850(\alpha_\ell - 1.0)^2$$  \hspace{1cm} (5c)
$$c_5 = +0.745 - 0.390(\alpha_\ell - 1.0) + 0.200(\alpha_\ell - 1.0)^2$$  \hspace{1cm} (5d)
$$c_6 = +1.628 - 0.110(\alpha_\ell - 1.0) + 0.600(\alpha_\ell - 1.0)^2$$  \hspace{1cm} (5e)

and for the dimer chain (with $J_1 = 1$) over the range $0.6 \lesssim \alpha_d \lesssim 0.8$ we found

$$c_2 = +8.145 - 61.76(\alpha_d - 0.7) + 406.3(\alpha_d - 0.7)^2$$  \hspace{1cm} (6a)
$$c_3 = +0.562 + 2.840(\alpha_d - 0.7) + 7.300(\alpha_d - 0.7)^2$$  \hspace{1cm} (6b)
$$c_4 = +0.456 - 0.435(\alpha_d - 0.7) + 1.750(\alpha_d - 0.7)^2$$  \hspace{1cm} (6c)
$$c_5 = +0.592 + 1.090(\alpha_d - 0.7) + 0.400(\alpha_d - 0.7)^2$$  \hspace{1cm} (6d)
$$c_6 = +1.663 + 0.160(\alpha_d - 0.7) - 1.40(\alpha_d - 0.7)^2$$  \hspace{1cm} (6e)

Due to the presence of large coefficients this parametrization is not useful far from the parameter ranges cited; if required the coefficients could be determined directly from the bulk-limit numerical results.
Our numerical results for the extrapolated bulk limit susceptibility of the ladder and dimer chain are shown in Figs.1 and 2 respectively, together with the interpolating functions defined by (4-6). The interpolating functions reproduce the bulk limit susceptibility with a typical accuracy of a few times $10^{-4}$ over the parameter ranges quoted above.

III. Comparison with the experimental $(VO)_2P_2O_7$ susceptibility

In a previous study Johnston et al. [9] presented results for the susceptibility of $(VO)_2P_2O_7$, and noted that the susceptibility of a dimer spin chain gives a very good description of the data for $\alpha_d \equiv J_2/J_1 = 0.7$ (fixed from an interpolation of theoretical curves for 0.6 and 0.8 from Refs. [11]), $J_1 = 11.32$ meV (hence $J_2 = 7.93$ meV) and $g = 2.00$. (Note that in our conventions the $\{J_n\}$ are twice as large as in Refs. [8] and [9].) A similar coupling of $J = 7.81$ meV was determined for VO(HPO$_4$)$_2 \cdot \frac{1}{2}$ H$_2$O, which consists of isolated V$^{+4}$ dimers, [10] and the $g$ factor of the V$^{+4}$ ion is known to be quite close to 2 from studies of other vanadium phosphates. [15] Of course it is not clear how the fitted dimer chain parameters relate to $(VO)_2P_2O_7$ if it proves to be a spin ladder.

To confirm these results we fitted our three-parameter ($J_1, \alpha_d, g$) dimer chain susceptibility, described by (4) and (6), to the data of Ref. [9], which consists of 606 values of $\chi(T)$ from $T = 7.2^\circ K$ to $344.34^\circ K$. We found the optimum parameter values to be $J_1 = 11.11$ meV, $\alpha_d = 0.722$ and $g = 1.99$. These are essentially the parameters found by Johnston et al., and the minor differences are presumably due to the systematic errors in interpolation (perhaps 1% in parameter values). The fitted dimer chain susceptibility and the data for $(VO)_2P_2O_7$ are shown in Fig.3.

We similarly fitted the three-parameter ($J_{||}, \alpha_\ell, g$) ladder susceptibility (4), (5) to the experimental $(VO)_2P_2O_7$ $\chi(T)$ data over the full temperature range. The optimum ladder parameters were found to be

\[ J_{||} = 7.76 \text{ meV} , \quad \alpha_\ell \equiv J_\perp / J_{||} = 1.007 , \]

(7a) (7b)
\[ g = 2.03 \]  

(7c)

The proximity of \( g \) to 2 provides a plausibility test of the fit, as does the fitted value of \( J_\perp = 7.82 \text{ meV} \), which is almost identical to the isolated-dimer \( J = 7.81 \text{ meV} \) found previously \[10\] in \( \text{VO(HPO}_4)_2\frac{1}{2} \text{H}_2\text{O} \). These results suggest that \( (\text{VO})_2\text{P}_2\text{O}_7 \) is very close to a uniform ladder \( (J_\perp = J_\parallel) \), which is presumably accidental because the rungs are bridged by two oxygens, whereas the chains have only single oxygens between \( \text{V}^{4+} \) ions. The fitted ladder \( \chi(T) \) is shown in Fig.4, and this model evidently also gives a very good description of the experimental data. The goodness of fit, defined by the residual

\[ f = \sum_i (\chi_{\text{expt.}}(T_i) - \chi_{\text{thy.}}(T_i))^2, \]

slightly favors the ladder model over the dimer chain. We cannot choose between the models definitively from the susceptibility data, however, because the variation in \( (\text{VO})_2\text{P}_2\text{O}_7 \) susceptibility estimated from samples with different annealing histories (Fig.1b of Ref. \[8\]) is somewhat larger than the difference between the predictions of the ladder and dimer chain models.

Finally, to test how well \( J_\perp \) and \( J_\parallel \) are determined, we studied the residual \( f \) in constrained two-parameter fits with \( g \) and \( J_\parallel \) variable but \( \alpha_\ell = J_\perp/J_\parallel \) fixed. As we changed \( \alpha_\ell \) from the optimum value 1.007 we found that by 0.90 and 1.12 the residual had increased by a factor of two. As we increase \( \alpha_\ell \) through the range \([0.9, 1.1]\) the fitted value of \( J_\parallel \) decreases from 8.2 meV to 7.3 meV, which can be taken as a conservative estimate of the accuracy to which \( J_\parallel \) is determined by the susceptibility. The fitted \( g \) factor remains close to 2.03 over this range. Outside this range of \( \alpha_\ell \) there is a rapid decrease in the quality of fit, reaching a factor of five increase in \( f \) by \( \alpha_\ell = 0.81 \) and 1.24.

**IV. Predictions of the ladder and dimer models**

Since we have determined ladder parameters for \( (\text{VO})_2\text{P}_2\text{O}_7 \) from our fit to the susceptibility, we can use the results of Ref. \[7\] to give predictions for the gap and spin-wave excitation spectrum. From Fig.2 of that reference we can see that the gap near \( J_\perp/J_\parallel = 1 \) is quite well determined by the Lanczos and Monte Carlo studies. An approximate linear interpolation gives
\[ \frac{E_{\text{gap}}}{J_{\parallel}} \bigg|_{\alpha_{\ell}=1} \approx 0.50(1) + 0.65 \left( \alpha_{\ell} - 1 \right), \] (8)

so for the optimum fitted parameters we predict

\[ E_{\text{gap}} = 3.9(1) \text{ meV}. \] (9)

Over the parameter range \( 0.9 \leq J_\perp/J_\parallel \leq 1.1 \) discussed above the predicted gap increases from 3.6 meV to 4.1 meV. \(^{10}\)

As was noted in Fig.3 of Ref. \(^{7}\), for \( J_\perp = J_\parallel \) the minimum energy required to excite a triplet spin wave on the ladder as a function of \( k \) closely resembles the dispersion relation of a spin-1/2 chain, except for the presence of excitation gaps. The lowest excitation is at \( k = \pi \), where the gap is \( \omega(\pi) = 0.50J_\parallel \), the maximum is shifted to a \( k < \pi/2 \), and a secondary minimum is at \( k = 0 \). This dispersion relation is symmetric about \( k = \pi \).

A complication not noted in Ref. \(^{7}\) is that the lowest-lying triplet spin-waves with these parameters arise from two distinct bands. The “primary” band, which contains the lowest gap, is odd under chain interchange \( (k_\perp = \pi) \), and is shown as solid lines for \( J_\perp/J_\parallel = 0.5, 1.0 \) and \( 2.0 \) in Fig.5. For large \( J_\perp \) these are excitations of a single rung, with energy \( \omega \approx J_\perp \). The “secondary” band (dashed lines in Fig.5) is even under chain interchange, and for large \( J_\perp \) these states consist of two excited rungs (hence \( \omega' \approx 2J_\perp \) and the even symmetry), with the two \( S = 1 \) excited rungs coupled to give \( S_{\text{tot}} = 1 \). Thus the secondary band may be interpreted as the excitation of two spin-wave quanta of the primary band. This interpretation leads us to anticipate several features of the secondary dispersion relation in the bulk limit, for example \( \omega'(k = 0) = 2\omega(k = \pi) \), so the band minimum of the secondary band in \((\text{VO})_2\text{P}_2\text{O}_7\) should lie at 7.8(2) meV given our parameters. One may similarly construct the entire secondary \( \omega'(k') \) given the primary \( \omega(k) \) (assuming there are no bound states), by finding the minimum-energy combination of two quanta with specified \( k' \).

In our representation in Fig.5 we fitted the function

\[ \omega(k) = [\omega(0)^2 \cos^2(k/2) + \omega(\pi)^2 \sin^2(k/2) + c_0^2 \text{sin}(k)^2]^{1/2}, \] (10)
which interpolates between the known analytic chain and dimer limits, to the 2x12 lattice data. (Except for the points $\omega'(k = 0)$ in the secondary band, which showed large finite size effects, and which we replaced as argued above by $2\omega(\pi)$.) For $J_\perp = J_{||} = J$ the fitted constants were found to be $\omega(0) = 1.890J$, $\omega(\pi) = 0.507J$ and $c_0 = 1.382J$. In Fig.6 we show the triplet dispersion relation which this parametrization predicts for $(\text{VO})_2\text{P}_2\text{O}_7$, together with a similar result for the secondary band, using the mean value $J_\perp = J_{||} = 7.79$ meV and the physical lattice spacing. The primary triplet band extends from 3.9 meV at $k = 0.813\text{A}^{-1}$ to 16 meV at about $0.3\text{A}^{-1}$, and then falls to 15 meV at $k = 0$. The secondary band extends from 7.9 meV at $k = 0$ to a broad plateau at an energy of about 17-18 meV centered on $k = 0.813\text{A}^{-1}$. Structure function calculations on the 2x12 lattice suggest that the secondary band should appear most clearly near the $k = \pi$ point ($0.813\text{A}^{-1}$).

For comparison we quote predictions for the triplet spin-wave dispersion relation in the dimer chain model. Of course the lattice spacing $a$ and the direction of the continuous momentum variable $k$ are problematical for $(\text{VO})_2\text{P}_2\text{O}_7$ in the dimer model because there is no obvious dimer chain interaction pathway. Since the dimer unit cell has length $2a$ the dispersion relation repeats with period $\Delta k = \pi/a$; this implies that the two different gaps we found for the ladder at 0 and $\pi/a$ are equal in the dimer chain. Another characteristic feature of the dimer chain dispersion relation is that it is symmetric about $\pi/2a$, due to inversion symmetry. For the parameters $J_1$, $J_2$ and $g$ found in our susceptibility fits the dimer chain model predicts a somewhat larger gap of $E_{\text{gap}} \approx 0.44J_1 = 4.9$ meV and a bandwidth of $\approx 11$ meV. It is interesting that one can apparently distinguish between the dimer chain and ladder models by an accurate measurement of the gap alone, using parameters derived from susceptibility fits.

V. Summary and Conclusions

In this paper we used numerical techniques to study the susceptibility of a Heisenberg antiferromagnetic spin ladder and a dimerized Heisenberg spin chain. We used exact numerical diagonalization to generate all energy eigenvalues and their degeneracies, which were then
used to determine $\chi(T)$ on ladders and dimer chains of up to 16 spins. We presented results for a range of temperatures and interaction ratios $J_{\perp}/J_{\parallel}$ (ladder) and $J_2/J_1$ (chain). These were extrapolated to give bulk limit estimates, which we parametrized using a function with five parameters. We fitted the bulk limit $\chi(T)$ to the susceptibility data for $(\text{VO})_2\text{P}_2\text{O}_7$, which is a candidate spin ladder system but is known to be accurately described by the dimer chain susceptibility. Our best fit to the dimer chain model accurately reproduces previous parameter values. Our best fit for the ladder is in slightly better agreement with the data, and indicates that $(\text{VO})_2\text{P}_2\text{O}_7$ has very similar $J_{\perp}$ and $J_{\parallel}$ values. With these parameters we give numerical predictions for the spin-wave excitation gap of $(\text{VO})_2\text{P}_2\text{O}_7$ and for other properties of the spin-wave dispersion relation.

VI. Acknowledgements

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[14] A fit of this form to the experimental susceptibility gave parameter values of $c_1 = 0.400$ cm$^3$ °K / mole V, $c_2 = 201.0$°K, $c_3 = 0.728$, $c_4 = 46.2°K$, $c_5 = 74.1°K$, and $c_6 = 1.750$. These values were not used in our fits to the ladder and dimer chain models and are quoted for reference only.

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| $T/J$ | 0.5  | 0.7  | 0.9  | 1.0  | 1.1  |
|------|------|------|------|------|------|
| 0.05 | .001034 | .000434 | .000095 | .000036 | .000012 |
| 0.10 | .024049 | .015862 | .007576 | .004697 | .002730 |
| 0.15 | .052841 | .040907 | .026020 | .019306 | .013692 |
| 0.20 | .071958 | .059399 | .043488 | .035436 | .027946 |
| 0.25 | .086240 | .073189 | .057624 | .049470 | .041489 |
| 0.30 | .098180 | .084851 | .069643 | .061651 | .053662 |
| 0.35 | .108058 | .094958 | .080161 | .072384 | .064535 |
| 0.40 | .115854 | .103404 | .089220 | .081722 | .074105 |
| 0.45 | .121734 | .110128 | .096743 | .089607 | .082308 |
| 0.50 | .125983 | .115240 | .102749 | .096035 | .089124 |
| 0.55 | .128895 | .118955 | .107366 | .101100 | .094615 |
| 0.60 | .130729 | .121508 | .110776 | .104954 | .098906 |
| 0.65 | .131696 | .123113 | .113171 | .107773 | .102151 |
| 0.70 | .131970 | .123957 | .114733 | .109728 | .104508 |
| 0.75 | .131691 | .124192 | .115617 | .110972 | .106127 |
| 0.80 | .130975 | .123942 | .115954 | .111638 | .107136 |
| 0.85 | .129917 | .123308 | .115852 | .111835 | .107648 |
| 0.90 | .128592 | .122373 | .115402 | .111656 | .107754 |
| 0.95 | .127064 | .121205 | .114674 | .111175 | .107534 |
| 1.00 | .125384 | .119856 | .113728 | .110454 | .107051 |
| 1.25 | .115891 | .111691 | .107134 | .104726 | .102238 |
| 1.50 | .106267 | .102995 | .099495 | .097661 | .095775 |
| 1.75 | .097456 | .094849 | .092086 | .090649 | .089174 |
| 2.00 | 0.89662 | 0.87541 | 0.85311 | 0.84156 | 0.82975 |
|------|---------|---------|---------|---------|---------|
| 2.25 | 0.82839 | 0.81084 | 0.79250 | 0.78303 | 0.77337 |
| 2.50 | 0.76876 | 0.75402 | 0.73867 | 0.73077 | 0.72274 |
| 2.75 | 0.71649 | 0.70394 | 0.69092 | 0.68424 | 0.67745 |
| 3.00 | 0.67046 | 0.65965 | 0.64848 | 0.64276 | 0.63695 |
| 3.25 | 0.62971 | 0.62031 | 0.61062 | 0.60566 | 0.60064 |
| 3.50 | 0.59344 | 0.58520 | 0.57671 | 0.57238 | 0.56799 |
| 3.75 | 0.56099 | 0.55370 | 0.54621 | 0.54239 | 0.53853 |
| 4.00 | 0.53181 | 0.52531 | 0.51866 | 0.51527 | 0.51184 |
TABLE II. $\chi(T)$ versus $T/J_1$ for the $N = 16$ dimer chain model.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
\text{T/J$_1$} & 0.2 & 0.4 & 0.6 & 0.7 & 0.8 & 1.0 \\
\hline
0.05 & .000000 & .000001 & .000032 & .000207 & .001380 & .011118 \\
0.10 & .000616 & .001530 & .006061 & .013706 & .031256 & .073202 \\
0.15 & .009732 & .015373 & .032088 & .049187 & .073849 & .105906 \\
0.20 & .035487 & .045476 & .067867 & .084726 & .103142 & .117932 \\
0.25 & .071654 & .081545 & .100186 & .111536 & .121656 & .124279 \\
0.30 & .107862 & .114179 & .125146 & .130670 & .134374 & .129372 \\
0.35 & .138004 & .139715 & .143241 & .144277 & .143674 & .134013 \\
0.40 & .160397 & .158026 & .155844 & .153834 & .150521 & .138121 \\
0.45 & .175673 & .170271 & .164219 & .160299 & .155375 & .141511 \\
0.50 & .185222 & .177821 & .169378 & .164351 & .158550 & .144073 \\
0.55 & .190459 & .181882 & .172110 & .166518 & .160317 & .145789 \\
0.60 & .192568 & .183407 & .173028 & .167222 & .160925 & .146707 \\
0.65 & .192465 & .183123 & .172604 & .166806 & .160003 & .146916 \\
0.70 & .190827 & .181567 & .171200 & .165544 & .159549 & .146517 \\
0.75 & .188146 & .179129 & .169092 & .163656 & .157931 & .145614 \\
0.80 & .184775 & .176099 & .166488 & .161314 & .155889 & .144304 \\
0.85 & .180966 & .172681 & .163547 & .158652 & .153537 & .142674 \\
0.90 & .176898 & .169028 & .160386 & .155772 & .150965 & .140797 \\
0.95 & .172699 & .165246 & .157093 & .152755 & .148245 & .138736 \\
1.00 & .168456 & .161412 & .153734 & .149660 & .145433 & .136543 \\
1.25 & .148209 & .142928 & .137255 & .134274 & .131202 & .124795 \\
1.50 & .130981 & .126962 & .122690 & .120461 & .118172 & .113424 \\
1.75 & .116819 & .113687 & .110382 & .108667 & .106912 & .103283 \\
2.00 & .105181 & .102682 & .100061 & .098707 & .097324 & .094474 \\
\hline
\end{tabular}
\end{table}
| 2.25 | .095528 | .093493 | .091370 | .090276 | .089161 | .086869 |
|------|---------|---------|---------|---------|---------|---------|
| 2.50 | .087431 | .085744 | .083990 | .083090 | .082173 | .080293 |
| 2.75 | .080559 | .079139 | .077668 | .076914 | .076147 | .074579 |
| 3.00 | .074663 | .073452 | .072201 | .071561 | .070912 | .069584 |
| 3.25 | .069555 | .068511 | .067434 | .066885 | .066327 | .065190 |
| 3.50 | .065090 | .064181 | .063245 | .062768 | .062284 | .061299 |
| 3.75 | .061157 | .060357 | .059537 | .059119 | .058696 | .057834 |
| 4.00 | .057666 | .056959 | .056233 | .055864 | .055491 | .054731 |