Random exchange effects in antiferromagnetic quantum spin chains: A Monte Carlo study

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We have carried out Monte Carlo studies of a random-exchange antiferromagnetic spin-$\frac{1}{2}$ chain. For systems with XY-like (anisotropic) and with Heisenberg (isotropic) coupling, our results confirm the existence of a disorder-induced low-temperature (T) divergence in the long-wavelength S^z-S^z susceptibility χ which was previously predicted by real-space renormalization-group (RSRG) treatments. Over the finite temperature range studied, these results are consistent with a $1/(T\ln^2 T)$ behavior of χ, and hence in qualitative agreement with the RSRG results. As in the XY-Heisenberg regime, we also find a disorder-induced enhancement of the low-T susceptibility for a system with Ising-like exchange coupling which, over the finite temperature range studied, is again consistent with RSRG results. However, there are inconsistencies between the RSRG predictions in the Ising-like regime at very low temperatures, and the exact results for the random-exchange Ising chain and the low-temperature behavior of χ in the Ising-like regime may in fact be more complicated than predicted by RSRG. Finally, we also present results for the antiferromagnetic susceptibility and structure factor. For both Heisenberg and Ising-like systems, we find that disorder suppresses the long-range antiferromagnetic correlations at low T.

I. INTRODUCTION

During recent years, one-dimensional (1D) disordered spin systems have received a great deal of theoretical attention.[1-6] Experimentally, this was stimulated, in part, by the unusual magnetic properties of certain tetracyanoquinodimethane (TCNQ) compounds.[7-10] For example, quinolinium $(TCNQ)_2$ is found to exhibit at low temperatures T a power-law divergence in the magnetic susceptibility,[7,10]

$$\chi \propto 1/T^{\alpha} , \tag{1}$$

where α is typically less than but close to unity.

The magnetic behavior of this material is commonly described as that of a quantum spin-$\frac{1}{2}$ chain[10] with a random and possibly anisotropic antiferromagnetic exchange coupling as given by the Hamiltonian

$$H=\frac{1}{2}\sum_{1\le j\le N} J_j(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\gamma\sigma_j^z\sigma_{j+1}^z) . \tag{2}$$

Here, N denotes the number of lattice sites, σ_j^x, σ_j^y, and σ_j^z are the Pauli matrices for a spin at a lattice site j, J_j denotes the exchange coupling between spins at sites j and $j+1$, and γ is the (site-independent) exchange anisotropy ratio. The J_j's are assumed to be randomly and independently distributed according to some probability distribution $P(J)$ [where $P(J)\equiv 0$ for $J<0$].

Several real-space renormalization-group (RSRG) treatments of (1) have been proposed which indeed indicate the possibility of a *disorder-induced* low-T divergence of the long-wavelength magnetic susceptibility.[3-6] Namely, for the Heisenberg case[3-6] ($\gamma=1$) and in the XY-like regime,[5] $0\le\gamma<1$, the RSRG results predict that in the presence of disorder the susceptibility exhibits a divergence of the form (1), however, with an exponent α that is slowly temperature dependent. More specifically, it was suggested that for $0\le\gamma\le 1$ and $T\to 0$, χ (as obtained from numerical solution of the RSRG equation) can be represented as[5]

$$\chi = A/[T\ln^m(T/T_0)] , \tag{3}$$

where the exponent m is close to 2 and only weakly dependent on γ or the distribution of exchange coupling. These results are in contradiction to an earlier cluster approximation treatment of the Heisenberg case ($\gamma=1$),[1] which predicted that $\chi(T)$ diverges at $T=0$ only if the distribution $P(J)$ has a corresponding singularity at $J=0$. They are consistent, however, with exact solutions of the XY case ($\gamma=0$), where it can be shown that, for arbitrarily weak disorder in the J_j's, χ exhibits a low-T divergence of the form (3) with an exponent $m=2$,[11,12] even for nonsingular distributions $P(J)$. Based on these results, it has been conjectured[5] that the $1/(T\ln^2 T)$ law might be the universal $T\to 0$ behavior of χ for $0\le\gamma\le 1$ and for arbitrary nonsingular distributions $P(J)$. However, the RSRG treatments[3-5] involve uncontrolled approximations so that a test of their reliability by comparison to numerical Monte Carlo (MC) results is of interest.

Aside from the long-wavelength properties, the effects of randomness on the long- and short-range antiferromagnetic (AF) order are of interest. Exact solutions[13-15] show that in the absence of disorder, the Hamiltonian (1) in the XY Heisenberg regime ($0\le\gamma\le 1$) exhibits a gapless excitation spectrum and AF spin-spin correlations at

$T=0$ decay algebraically, e.g., with a power law as a function of distance in real space. In the Ising-like regime ($\gamma>1$), a finite gap, Δ, appears in the spectrum and the ground state exhibits long range AF order, e.g., AF spin-spin correlations that approach a nonzero constant at large distances. For nonzero temperatures, the algebraic ($0\le\gamma\le1$) or long-range ($\gamma>1$) correlations are damped exponentially at large distances with a finite correlation length ξ. As $T\to0$, ξ diverges in a power-law fashion if $0\le\gamma\le1$ and exponentially, like $\exp(\Delta/T)$, if $\gamma>1$.

In the presence of disorder, an exact solution has been obtained only for the Ising limit ($\gamma\to\infty$) of (2).[16,17] Although randomness does not destroy the long-range order of the ground state in the Ising chain, it does reduce the gap in the excitation spectrum. In fact, if the distribution $P_z(J^z)$ of the random σ^z-σ^z couplings J_j^z, extends to arbitrarily small values of J^z, the spectrum is gapless. At low but finite temperatures, the suppression of the gap, in turn, reduces the long-range spin-spin correlations, i.e., the magnitude as well as the strength of the low-T divergence of the correlation length ξ.[18] One would expect to observe similar effects for the quantum spin system (2). In fact, preliminary MC results for the Heisenberg case[19] indicated that disorder tends to suppress the AF spin-spin correlations at large distances.

In the present paper, we report a more detailed MC study of both the long-wavelength and the AF (short-wavelength) spin-spin correlation functions and susceptibilities of (2). Section II contains a brief outline of the MC procedure. In Sec. III, we discuss the results obtained for the long-wavelength susceptibility and compare them to the RSRG results. We also present results for the AF spin-spin susceptibilities and correlations. A summary is given in Sec. IV.

II. NUMERICAL METHODS

We have used the world-line (WL) algorithm[20] to simulate the disorder averaged longitudinal susceptibility and static structure factor at wave vector q,

$$\chi(q)=\frac{1}{N}\int_0^\beta d\tau\overline{\langle S_q^z(\tau)S_{-q}^z(0)\rangle}\ ,$$
$$S(q)=\frac{1}{N}\langle S_q^z(0)S_{-q}^z(0)\rangle\ . \tag{4}$$

Here, $\beta=1/T$ is the inverse temperature, $\langle\cdots\rangle$ and $\overline{\cdots}$ denote the thermal and the disorder average, respectively, and

$$S_q^z(\tau)=\tfrac{1}{2}\sum_l\exp(-iql+H\tau)\sigma_l^z\exp(-H\tau)$$

is the q component of the magnetization at imaginary time τ. The exchange couplings J_j were chosen randomly for each bond $(j,j+1)$ according to a rectangular distribution of width $2\Delta J$,

$$P(J)=1/(2\Delta J),\quad |J-1|<\Delta J \tag{5}$$

and vanishing otherwise. [Here, we have set the energy units such that $P(J)$ is centered around $\overline{J}_j\equiv1$.]

The disorder averages were obtained by performing MC measurements on typically 20—50 different J_j configurations (depending on lattice size). For each J_j configuration, 1000—2000 WL configurations[20] were sampled, each of them generated from the preceding one by at least ten updating sweeps through the space-time lattice.[20] The number of time slices[20] L was typically chosen such that $\Delta\tau\equiv\beta/L=0.2$ for the measurements reported here. Notice that for any finite value of $\Delta\tau$ our WL results will exhibit a systematic error that vanishes only in the limit of infinite L (with β fixed). For certain quantities, measured with sufficiently large (i.e., too large) values of $\Delta\tau$, this error can become significantly larger than the statistical error (of typically a few percent), as has recently been found[21] by comparing such world-line data for the $q=\pi$ structure factor of the one-dimensional 1D Heisenberg chain with exact solutions for this model. We have therefore carried out additional measurements with $\Delta\tau=0.1$ for a few parameter values β, γ, and ΔJ to determine the magnitude of such systematic errors due to this finite $\Delta\tau$ effect. Within statistical error (typically less than 5% for $T>0.2$ and of the order of 10—15% for $T<0.2$), the results for $\chi(q)$ did not show any detectable $\Delta\tau$ dependence. We conclude, therefore, that for the data presented below, this systematic error is less than the statistical error. An additional test for such systematic errors is provided for the case $\gamma=0$, by comparing the WL data to those obtained with the "real-frequency" method[22] described below. As shown in Fig. 1(a), these data are in satisfactory agreement.

Since the WL algorithm evaluates thermal averages in an ensemble with a fixed total magnetization ($S_{q=0}^z=\text{const}$),[20] we cannot determine χ at $q=0$. To obtain the long-wavelength susceptibility, we have therefore measured χ at the smallest possible nonzero values that q may attain in an N-site system, namely at $q=2\pi/N$, $4\pi/N,\ldots,2\pi m/N$ with $m\ll N$. To study the AF order in the presence of randomness, we have measured $S(q)$ and $\chi(q)$ at and in the vicinity of $q=\pi$. The spatial lattice size, N, in our simulations was chosen proportional to the inverse temperature, such that $\beta/N=0.2$. In addition, measurements were taken with $\beta/N=0.1$ and with a constant $N=160$ for several values of the parameters β, γ, and ΔJ. Since the different values of $\chi(q)$ for q small thus obtained agree within statistical error (typically a few percent at high temperatures and of the order of 10—15% at low T), we believe that the finite-size effects are negligible in our long-wavelength results. Furthermore, for $N>20$ we find (within statistical error) no difference between the $\chi(q)$ values at $q=2\pi/N$ and $4\pi/N$. We are therefore confident that these values represent accurate estimates of $\chi(q=0)$. The WL calculations were carried out on an IBM 3081 computer. For the largest lattice sizes studied, $N\times L=140\times140$ (i.e., $\beta=28$) a typical run consisting of 200 000 lattice sweeps took of the order of 6 h of CPU time.

Finally, in the XY ($\gamma=0$) limit, a Jordan-Wigner transformation maps Eq. (2) onto a 1D system of noninteracting spinless fermions with a random one-electron transfer J_j. The susceptibility χ, Eq. (4), is then given by

$$\chi=\beta\int_{-\infty}^{\infty}d\omega f(\omega)[1-f(\omega)]N(\omega)\ , \tag{6}$$

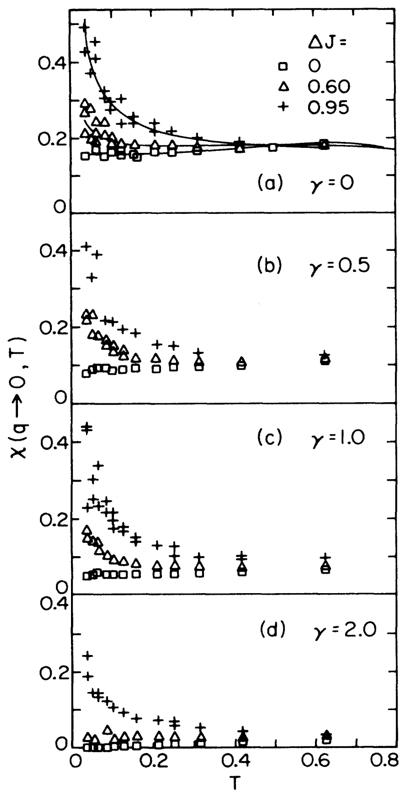

FIG. 1. Long-wavelength magnetic susceptibility $\chi(q\to 0,T)$ as a function of temperature T for several values of disorder strength ΔJ and anisotropy ratio γ. In (a) the "real frequency" MC results (Ref. 22) are shown as a solid line. All other data are WL MC results.

where $N(\omega)$ is the fermion single-particle-energy density of states, and $f(\omega)=(e^{\beta\omega}+1)^{-1}$ is the Fermi function. For the pure case in which $\Delta J=0$ with $J=1$ one has

$$N(\omega)=\frac{1}{2\pi[1-(\omega/2)^2]^{1/2}} . \tag{7}$$

In this case, the susceptibility remains finite as $T\to 0$, approaching the density of states at the Fermi surface $N(0)$

$$\chi\sim\frac{1}{2\pi}\left[1+\frac{\pi^2}{12}T^2\right],\quad T\ll 1 \tag{8}$$

while for large T

$$\chi\sim\frac{1}{4T},\quad T\gg 1 . \tag{9}$$

In the presence of a random XY exchange J, it was shown by Dyson[11] that

$$N(\omega)\sim\frac{A}{\omega\ln^3(\omega/\omega_0)} . \tag{10}$$

This leads to a divergence in the low-temperature behavior of χ of the form given by Eq. (3) with $m=2$ and $T_0=\omega_0$.

For the XY ($\gamma=0$) limit, alternative numerical techniques are also available. For example, one can simply evaluate an average $N(\omega)$ by an exact diagonalization of the N-site free-electron Hamiltonian

$$H=\sum_i (J_i C_{i+1}^{\dagger}C_i+\text{H.c.}) \tag{11}$$

with J_i distributed according to $P(J_i)$. We have done this for $N=140$, averaging over 50 configurations giving results for $\chi(T)$ with a statistical accuracy of a few percent for $0.1<T<4$. The lower limit on T is set by the length of the chain. In order to extend this numerical treatment of the XY ($\gamma=0$) system to lower temperatures, we have adapted a real frequency Monte Carlo technique introduced by Hirsch and Eggarter[22] to determine $N(\omega)$. Here the effective length of the lattices ranged up to 10^4 sites, and the results agreed with those obtained with exact diagonalization in the high-temperature regime.

III. RESULTS AND DISCUSSION

In Fig. 1(a), we show the WL data from several different MC runs for $\gamma=0$ together with the results obtained from the real frequency simulation. They are in good agreement with each other and with the exact diagonalization results [not displayed in Fig. 1(a)]. Whereas, in the homogeneous system ($\Delta J=0$), χ approaches a constant as $T\to 0$, the low-temperature divergence is clearly developed below $T\sim 0.2$ in the disordered systems. To check whether χ has the expected $1/(T\ln^2 T)$ behavior,[5,11,12] it is convenient to plot $(T\chi)^{-1/2}$ versus $\log_{10}T$, as shown in Fig. 2(a). Indeed, the data points for the disordered systems fall on a straight line, whereas for the homogeneous case, they exhibit an upward curvature.

In Figs. 1(b)—1(d) and 2(b)—2(d) the analogous data are shown for nonzero values of γ. Note that the XY-like ($\gamma=0.5$) and the Heisenberg ($\gamma=1$) system seem to behave qualitatively in the same way as the XY system: Without disorder χ approaches a nonzero constant; in the presence of disorder, it increases as $T\to 0$. Considering the limited temperature range and statistical accuracy of our WL data, we should caution, however, that these results do not establish any proof for a universal $1/(T\ln^2 T)$ divergence of χ for $T\to 0$. For example, within the limits of accuracy our WL MC results would also be consistent with a simple power law. Let us emphasize that a power law ($1/T^{\alpha}$, with α close to unity) and a $1/(T\ln^2 T)$ law are very similar. They can be distinguished only by accurate measurements over many orders of magnitude in T. With our present WL MC methods, such measurements would require prohibitively long simulation times. Nevertheless, our results confirm at least qualitatively the RSRG prediction that $\chi(q=0)$ is divergent at $T=0$.

The data for an Ising-like system are shown in Figs. 1(d) and 2(d). In the homogeneous system, χ vanishes as $T\to 0$. In the moderately disordered system ($\Delta J=0.6$) it is roughly constant and nonzero over the temperature range studied; finally, in the strongly disordered system ($\Delta J=0.95$), the data show the same increasing behavior (as $T\to 0$) that is observed in the XY-like and Heisenberg regime ($0\le\gamma\le 1$). By comparison, the RSRG treatment[5]

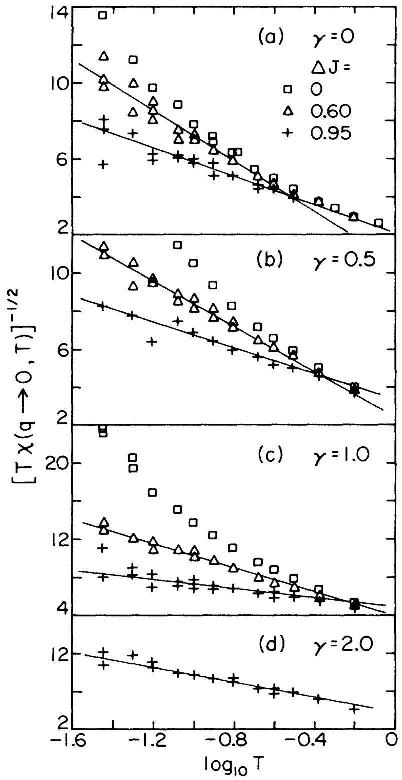

FIG. 2. WL MC data from Fig. 1 plotted as $(T\chi)^{-1/2}$ vs $\log_{10}T$. In the presence of disorder ($\Delta J\neq 0$), the data at low T fall on a straight line (——), indicated as a guide to the eye.

predicts that for $\gamma>1$ and with a nonsingular, sufficiently broad $P(J)$ [e.g., for $\Delta J\to 1$ in Eq. (5)], χ should first increase with decreasing T as in the Heisenberg XY regime ($0\leq\gamma\leq 1$) until it reaches a maximum at some temperature T_m and then decrease to zero for $T_m>T\to 0$. For our parameter values, $\Delta J=0.95$ and $\gamma=2$, one can estimate (from the RSRG results[5] obtained for $\Delta J=1.0$) an upper bound for T_m of the order of 10^{-3} or less which is out of the range of our WL MC method. Hence, in the temperature range studied, our data are consistent with the available RSRG results.[5] However, they do not allow any conclusions regarding the very low-temperature behavior, namely the question whether χ exhibits a maximum and decreases to zero at very low T.

In this connection, it is worthwhile pointing out that the low-temperature RSRG predictions[5] $\Delta J=1$ seem to be inconsistent with the exact solution[16–18] for the random exchange Ising chain ($\gamma\to\infty$). To discuss this it is convenient to parametrize the system in terms of the σ^z-σ^z exchange couplings, J_j^z, instead of the XY couplings

$$J_j\equiv J_j^z/\gamma \tag{12}$$

so that for finite γ, $P(J)$ is given in terms of the distribution of J_j^z's, $P_z(J^z)$,

$$P(J)=\gamma P_z(\gamma J)\ . \tag{13}$$

We then consider the limit $\gamma\to\infty$ for fixed J_j^z with $\bar{J}^z=1$ and hence all $J_j\to 0$. The exact Ising result for χ vanishes at $T=0$ if

$$P_z(J^z)=0,\quad 0\leq J^z<\Delta_P\ , \tag{14}$$

where Δ_P denotes a finite gap in the distribution P_z around $J^z=0$. However, if

$$\lim_{J^z\to 0} P_z(J^z)>0 \tag{15}$$

[for example, for a distribution of the form (5) with a half width $\Delta J^z=1$] the Ising susceptibility approaches a nonzero value as $T\to 0$. One would expect that this result [i.e., $\lim_{T\to 0}\chi(q\to 0,T)>0$ if $\lim_{J_z\to 0}P_z(J^z)>0$] remains unchanged if a small XY contribution is added to the pure Ising Hamiltonian (i.e., $\gamma\gg 1$, but finite), since the quantum term generally tends to enhance fluctuations and hence $\chi(q=0)$ in an antiferromagnetically coupled system. The RSRG approach,[5] on the other hand, predicts that χ vanishes as $T\to 0$ for a distribution of type (15).

In line with these remarks, it is important to note that the RSRG treatment[5] has a general tendency to overestimate the gap in the excitation spectrum, as pointed out already in Ref. 5. As a consequence, it underestimates the low-temperature susceptibility. For example, for a Heisenberg chain ($\gamma=1$) without disorder, RSRG leads to a vanishing χ at $T=0$, in disagreement with our MC results [Fig. 1(c)] as well as earlier exact diagonalizations[23] of finite-size chains which indicate that χ is finite and nonzero at $T=0$.

These observations raise the interesting question as to whether the low-T behavior in the Ising-like regime may in fact be more complicated than suggested by the RSRG approach.[5] Although χ certainly vanishes at $T=0$ in an Ising system with $\Delta_P>0$ [Eq. (14)], this may not be true any more in the presence of a sufficiently strong XY term: Note that for a strongly disordered Ising system with a very small gap Δ_P in the distribution $P_z(J^z)$, also the gap in the excitation spectrum,

$$\Delta=2\Delta_P \tag{16}$$

is small (compared to the average exchange coupling $\bar{J}^z$, say). If we now introduce an XY term with an average strength $\bar{J}\equiv\bar{J}_z/\gamma$ it may well be possible that the gap in the excitation spectrum vanishes if $\bar{J}$ becomes of the order of or larger than Δ_P. This, in turn, will change the low-temperature behavior of χ from an $\exp(-\Delta/T)$ dependence to something like a power law. It can in fact lead to a nonzero, even divergent, value of χ at $T=0$.

To be specific, let us consider the class of distributions $P_z(J^z)$ of the form (5) with a half width ΔJ^z. The Hamiltonian is then parametrized by the two quantities γ and $\alpha=\Delta J^z/\bar{J}^z$. One can construct a ground-state phase diagram in the α-γ plane with phase boundaries that separate different regions characterized by

$$\chi_0\equiv\lim_{T\to 0}\chi(q=0) \tag{17}$$

being either zero, infinite, or nonzero and finite. The RSRG phase diagram is shown in Fig. 4(a): There is one phase boundary at $\gamma=1$ which separates the XY Heisen-

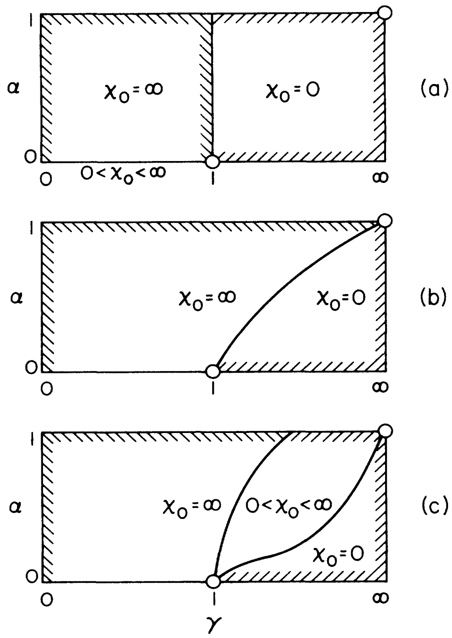

FIG. 3. Susceptibility ground-state phase diagram of H, Eq. (2), in terms of anisotropy γ and disorder strength $\alpha=\Delta J/\bar{J}$. (a) RSRG prediction; (b) and (c) possibilities suggested in text.

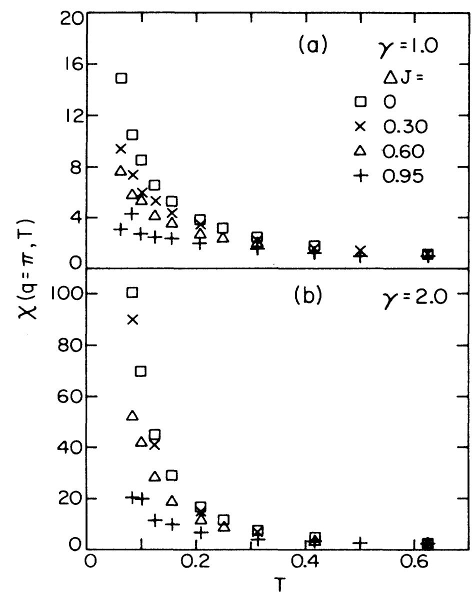

FIG. 4. Antiferromagnetic susceptibility $\chi(q=\pi)$ as a function of temperature T for several values of disorder strength ΔJ, Eq. (5), and anisotropy ratio γ.

berg regime, $0\leq\gamma\leq1$, with $\chi_0=\infty$ from the Ising-like regime, $\gamma>1$, where $\chi_0=0$. Based on the foregoing discussion, we suggest that other possibilities, sketched schematically in Figs. 3(b) and 3(c), cannot be ruled out. First of all, sufficiently strong fluctuations and disorder may lead to a region of infinite χ_0 extending into the Ising-like regime, as indicated in Fig. 3(b). Furthermore, it is possible that the region of infinite χ_0 may be separated from the $\chi_0=0$ region by an intermediate phase where $0<\chi_0<\infty$. In concluding our discussion of the $q=0$ susceptibility, let us emphasize that our MC results for $\gamma=2$ [Figs. 1(d) and 2(d)] are not inconsistent with these possibilities.

We now turn to a brief discussion of the effects of randomness on the antiferromagnetic order. In Figs. 4 and 5, we show WL data of the T dependence of the susceptibility $\chi(q=\pi)$ and the structure factor $S(q=\pi)$, respectively, for values of $\gamma=1$ and $\gamma=2$. In both quantities, one observes a suppression of the low-temperature divergence with increasing disorder strength. Also note the difference in the scale of both χ and S between the Heisenberg $(\gamma=1)$ and the Ising-like $(\gamma=2)$ system. The suppression in the low-T divergence is accompanied by a reduction of the AF correlation length. In Fig. 6, we have displayed the q dependence of $S(q)$ near $q=\pi$ for a disordered $(\Delta J=0.6)$ and a homogeneous 60-site system $(\Delta J=0)$ at an inverse temperature $\beta=12$. In the Heisenberg case [Fig. 6(a)], the correlation length ξ (roughly the inverse width of the peak at $q=\pi$) at this temperature is less than the system size both for the disordered and the homogeneous system. As expected, the peak at $q=\pi$ is broadened (i.e., ξ is reduced) by the disorder. In the Ising-like case [Fig. 6(b)], on the other hand, the correlation lengths are much larger than the system size as evidenced by a jump in $S(q)$ by almost 1 order of magnitude as we go from $q=\pi-2\pi/N$ to $q=\pi$. Nevertheless, the broadening of the peak at $q=\pi$ due to the disorder can still be observed in the wings of the peak (at $q=\pi-1\pi/N$, $\pi-4\pi/N,\ldots$). These data are qualitatively similar to the results for various exactly solvable

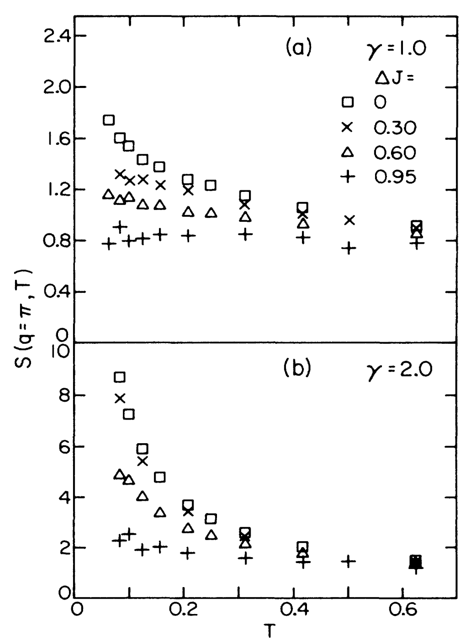

FIG. 5. Structure factor $S(q=\pi)$ as a function of temperature T for several values of disorder strength ΔJ and anisotropy ratio γ. All data shown are WL MC results.

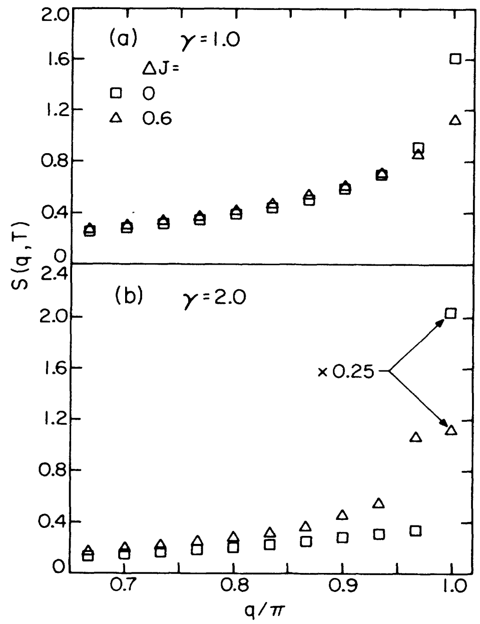

FIG. 6. Structure factor $S(q)$ as a function of wave vector q at temperature $T=\frac{1}{12}$ for a homogeneous ($\Delta J=0$) and a disordered system ($\Delta J=0.6$) and different anisotropy ratios γ.

random spin chains,[18] where an analogous suppression of the long-range correlations is found.

IV. SUMMARY

In conclusion, our MC results confirm that disorder can give rise to a low-temperature divergence in the long-wavelength ($q=0$) susceptibility χ of an XY-like ($0\leq\gamma<1$) or Heisenberg ($\gamma=1$) antiferromagnetic quantum spin chain. In the temperature range studied, they are consistent with recent RSRG results,[3–6] in particular, with a $1/(T\ln^2 T)$ dependence of χ as $T\rightarrow 0$. We have also pointed out certain inconsistencies in the RSRG results[5] for the low-T behavior in the Ising-like regime ($\gamma>1$). We discuss alternative phase diagrams for this regime which are consistent with our MC data and the Ising limit. Finally, we have studied the AF susceptibility $\chi(q=\pi)$ and structure factor $S(q=\pi)$ of a Heisenberg and an Ising-like system in the presence of disorder. We find that in both cases randomness tends to reduce the AF correlation length and hence $\chi(q=\pi)$ and $S(q=\pi)$.

We should mention at this point a recent publication[24] which proposes an "exact" numerical treatment of 1D quantum spin systems. Based on the "checkerboard" breakup,[20] the method is, in principle, applicable to the random exchange Hamiltonian (2).

While this work was being completed, we received the results of an analogous WL MC study[25] of the Hamiltonian (2) for the Heisenberg case $\gamma=1$. The data for the T dependence of $\chi(q\rightarrow 0)$ and $\chi(q=\pi)$ in Ref. 24 are, essentially, in agreement with the ones presented here.

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