Monte Carlo Study of Correlations in Quantum Spin Ladders

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We study antiferromagnetic spin-1/2 Heisenberg ladders, comprised of n_c chains ($2 \leq n_c \leq 6$) with ratio $J_\perp/J_\parallel$ of inter-chain to intra-chain couplings. The correlation length $\xi(T)$ is deduced from measurements of the correlation function. For even n_c, the static structure factor exhibits a peak at a temperature below the corresponding spin gap. Results for isotropically coupled ladders ($J_\perp/J_\parallel = 1$) are compared to those for the single chain and the square lattice. For $J_\perp/J_\parallel \leq 0.5$, the correlation function of the two-chain ladder is in excellent agreement with analytic results from conformal field theory, and $\xi(T)$ exhibits simple scaling behavior. [S0031-9007(96)01017-4]

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Low-dimensional quantum Heisenberg antiferromagnets (QHA) exhibit many fascinating properties. In 1931, Bethe demonstrated for the one-dimensional (1D) spin $S = 1/2$ nearest-neighbor Heisenberg chain that quantum fluctuations prevent the existence of an ordered ground state [1]. Instead, this system exhibits power-law correlations with gapless excitations. Haldane suggested in 1983 that all non-integer-spin chains are gapless, but that integer-spin chains should have a spin gap [2]. By now there is much evidence for the correctness of this famous conjecture [3]. For the two-dimensional (2D) analog of the spin chains, the square-lattice nearest-neighbor QHA, it has been established over the past decade that an ordered ground state exists even in the extreme quantum limit of $S = 1/2$ [4].

Spin ladders are arrays of coupled chains and thus present interpolating structures between 1D and 2D [5]. These systems are thought to be realized, with $S = 1/2$, in the materials $(VO)_2P_2O_7$ [6] and $Sr_{n-1}Cu_{n+1}O_{2n}$ [7]. They allow the study of the dimensional crossover from the power-law correlations of the $S = 1/2$ chain to the long-range order of the square lattice. Interestingly, ladders with an odd number n_c of chains have power-law spin correlations in their ground state, while those with even n_c exhibit exponentially decaying correlations due to the presence of a spin gap [5]. In analogy to the general S chain [2], the fundamental difference between even and odd ladders is thought to be of a topological nature [8,9].

In this Letter, isotropically coupled ladders as well as the two-chain ladder in the regime of weak inter-chain coupling are investigated. The former systems are directly relevant to the known experimental systems which are approximately isotropic [5]. Moreover, the crossover from 1D to 2D is most naturally studied in this case. Numerical simulations to determine both the correlation length and the static structure factor down to very low temperatures are performed. Our results provide a basis for comparison with future neutron scattering and NMR experiments. The two-chain ladder at weak inter-chain coupling allows us to investigate the formation of a spin gap away from the unstable $T = 0$ fixed point of the gapless $S = 1/2$ chain [10], and indeed serves to demonstrate the extreme fragility of the $S = 1/2$ chain power-law correlations. Our data for the low-temperature correlation function are in excellent agreement with a recent theoretical prediction [11]. Moreover, we discover that in this regime the correlation length exhibits universal scaling behavior with respect to the inter-chain coupling.

The Hamilton operator for a Heisenberg system of n_c $S = 1/2$ chains forming a ladder is

$$H = J_\parallel \sum_{\langle ij \rangle_\parallel} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle ij \rangle_\perp} \mathbf{S}_i \cdot \mathbf{S}_j \,. \tag{1}$$

Here, $\mathbf{S}_i = \frac{1}{2}\boldsymbol{\sigma}_i$ is the quantum spin operator at site i, while $\langle ij \rangle_\parallel$ and $\langle ij \rangle_\perp$ denote nearest neighbors along and between chains, respectively. The couplings considered are antiferromagnetic, that is $J_\parallel, J_\perp > 0$, and periodic boundary conditions are employed along the chains. We use units in which the lattice constant $a = 1$, $\hbar = k_B = 1$ and, unless noted otherwise, $J_\parallel = 1$.

The ladder systems are investigated with a very efficient loop cluster algorithm [12,13] which allows access to very low temperatures and the implementation of improved estimators in order to reduce statistical errors of observables. The simulated lattices are large enough, both along the chains and in Euclidean time, so that finite-size and finite Trotter number effects are comparable to the statistical errors. In particular, the length of the ladders is kept $\sim$15 times larger than the correlation length. Typically, 4×10^4 loop updates are performed for equilibration, followed by 4×10^5 measurements.

In order to obtain information about the gap $\Delta(n_c, J_\perp)$ for even n_c, we measure the uniform susceptibility

$$\chi(n_c, J_\perp; T) \sim T^{-1} \left\langle \left(\sum_i S_i^z \right)^2 \right\rangle . \tag{2}$$

Gap values extracted from fits to the low-temperature form [14]

$$\chi(n_c, J_\perp; T) \sim T^{-1/2} e^{-\Delta(n_c, J_\perp)/T} \tag{3}$$

are shown in Fig. 1. For $J_\perp \geq 2$, we find very good agreement with strong-coupling expansion results for

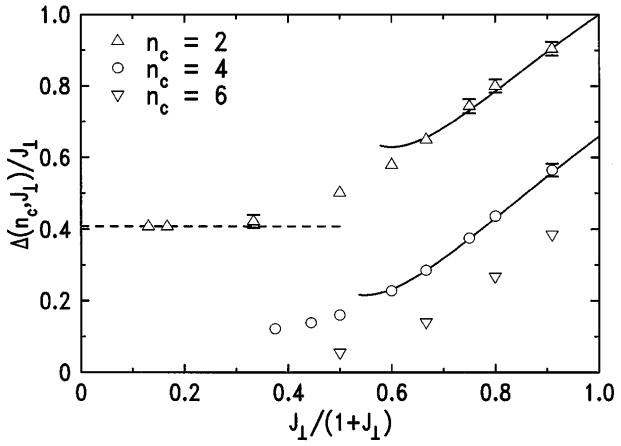

FIG. 1. Inter-chain coupling dependence of the spin gap. The solid lines are from Ref. [15], and the dashed line indicates the weak-coupling behavior $\Delta(2, J_\perp \to 0) = 0.41(1) J_\perp$.

$n_c = 2$ and 4 [15], shown as solid lines. Our susceptibility data for the isotropically coupled ladders ($J_\perp = 1$) agree well with recent Monte Carlo work [16], and we obtain $\Delta(n_c, 1) = 0.502(5), 0.160(5)$, and $0.051(6)$ for $n_c = 2, 4$, and 6, respectively. In an earlier study [8], $\Delta(2, 1) = 0.504$ and $\Delta(4, 1) = 0.190$ were found. For $n_c = 2$, we are able to access the weak-coupling regime characterized by $\Delta(2, J_\perp) \sim J_\perp$ [11,17]. We find $\Delta(2, J_\perp)/J_\perp = 0.41(1)$, which agrees with the value 0.42 found recently [18], but is somewhat smaller than $\Delta(2, J_\perp)/J_\perp = 0.47$ obtained previously [17]. It should be noted that our data do not allow us to discern any predicted logarithmic corrections [11,19] to the behavior $\Delta(2, J_\perp) \sim J_\perp$.

Next we compute the staggered correlation function

$$C(i, j) = \mathrm{sgn}(i, j) \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle, \tag{4}$$

where $\mathrm{sgn}(i, j)$ is 1 (-1) if the spins at i and j are separated by an even (odd) number of couplings. For two weakly coupled chains at $T = 0$, conformal field theory predicts [11]

$$C(r) = G_+(r) G_-(r) [G_-(r) G_-(3r) \pm G_+(r) G_+(3r)], \tag{5}$$

and this form is claimed to be exact in the continuum limit. The sign of the last term is plus for intra-chain and minus for inter-chain correlations, and r measures the distance of two spins along the ladder. The functions

$$G_\pm(r) = r^{-1/4} F_\pm(r/\xi)[1 \pm 2^{-3/2} \xi^{-1}] + \mathcal{O}(r^{-5/4}) \tag{6}$$

are correlation functions of the 2D Ising model, with scaling functions $F_\pm$ [20]. In Eq. (6), ξ denotes the spin-spin correlation length of the ladder system. The intra-chain and inter-chain correlation functions differ only at short distances. At large distances $r/\xi \gg 1$, $C(r)$ decays as

$$C(r) \sim r^{-\lambda} e^{-r/\xi} \tag{7}$$

with $\lambda = 1/2$, which is equivalent to the 2D Ornstein-Zernike (OZ) form. Figure 2 shows the low-temperature correlation function for $n_c = 2$ at a weak coupling of $J_\perp = 0.2$. The lines are the result of a fit to Eq. (5) with only two fitting parameters: ξ and an overall amplitude. The fit is excellent over the entire range and yields $\xi = 19.4(2)$. As is evident from Fig. 2, Eq. (5) correctly captures the crossover from the short- to the long-distance behavior with a concomitant change in length scales by a factor of ~ 3.

In order to deduce $\xi(n_c, J_\perp; T)$ for general $n_c, J_\perp$, and T, $C(i, j)$ is fit at large distances $r \geq 3\xi$ to the asymptotic form Eq. (7). For $n_c = 4$ and 6, Eq. (7) with $\lambda = 0.5$ describes the low-temperature data very well. However, we find that the asymptotic behavior for even n_c crosses over between $T \approx 0.2\Delta(n_c, J_\perp)$ and $T \approx 0.4\Delta(n_c, J_\perp)$ to the 1D OZ form, that is, $\lambda = 0$. For odd n_c, on the other hand, the 1D form works very well at all temperatures.

In Figure 3, the result of this analysis for $J_\perp = 1$ is shown together with $\xi(T)$ for the square lattice as obtained by both Monte Carlo [21] and neutron scattering in $Sr_2CuO_2Cl_2$ [4]. Because of the presence of a gap for even n_c, $\xi(T)$ remains finite as $T \to 0$. We estimate that $\xi(n_c, 1; 0) = 3.24(5)$ and 10.3(1) for $n_c = 2$ and 4, respectively. The result for $n_c = 2$ agrees with the value $\xi = 3.19(1)$ obtained previously [8]. However, in Ref. [8] $\xi = 5$ to 6 was obtained for $n_c = 4$, which is significantly smaller than our result. For $n_c = 2$ and 4 we obtain the respective velocities $c(n_c, 1) = \Delta(n_c, 1)\xi(n_c, 1; 0) = 1.63(2)$ and 1.65(3), which lie in between the 1D and 2D values $c_{1D} = \pi/2 \simeq 1.57$ and $c_{2D} \simeq 1.68$.

The correlation length of the single $S = 1/2$ chain has been determined in a thermal Bethe-ansatz study [22]:

$$\xi_{1D}^{-1}(T) \simeq T\Big[2 - b^{-1}\Big(1 - 0.486 b^{-1} \ln(b)\Big)\Big], \tag{8}$$

with $b = -\ln(0.3733T)$. For $T \leq 0.3$ our data for the chain agree with this low-temperature form, indicated by

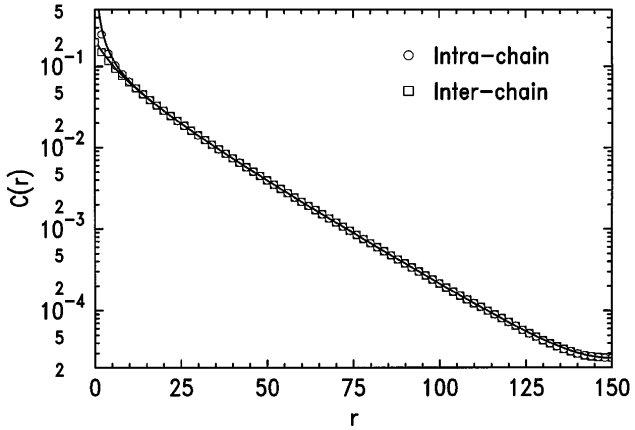

FIG. 2. Correlation functions at $T = 0.01$ for a $S = 1/2$ two-chain Heisenberg ladder of length 300 with $J_\perp = 0.2$. Periodic boundary conditions were employed along the chains, and for clarity $C(r)$ is shown only for even r. The lines are the result of a fit to Eq. (5) in the symmetrized form $[C(r) + C(300 - r)]$.

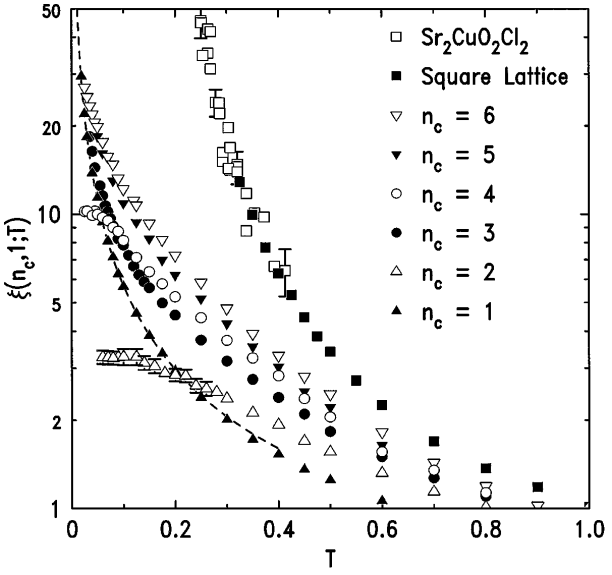

FIG. 3. Correlation length of n_c isotropically coupled antiferromagnetic $S = 1/2$ chains. The result for the single chain ($n_c = 1$) is compared with the theoretical prediction Eq. (8) (dashed line). Also shown are the results for the square lattice obtained from both Monte Carlo simulations [21] as well as neutron scattering experiments in $Sr_2CuO_2Cl_2$ [4].

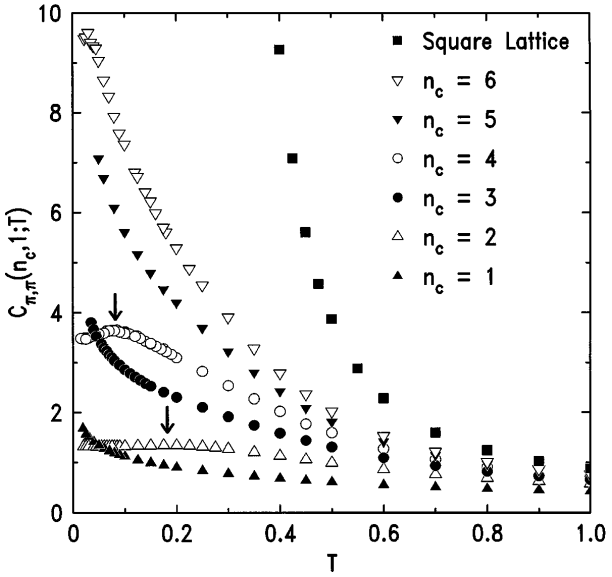

FIG. 4. Static structure factor at (π, π) for isotropically coupled antiferromagnetic $S = 1/2$ ladders, as well as for the single chain ($n_c = 1$) and the square lattice [21]. For even n_c, $C_{\pi,\pi}$ exhibits a peak (indicated by arrows) at a temperature below that corresponding to the relevant spin gap.

the dashed line in Fig. 3. We find that with decreasing temperature ξ for $n_c = 3$ and 5 gradually approaches ξ_{1D}.

In Figure 4 the static structure factor at (π, π), $C_{\pi,\pi} = \sum_{i,j} C(i,j)$, is shown for the isotropically coupled systems. The overall trend with n_c is similar to that for ξ. However, $C_{\pi,\pi}(n_c, J_\perp; T)$ for even n_c exhibits a peak at a temperature $T_{\max}$ well below the corresponding spin gap. Not surprisingly, $T_{\max}$ appears to coincide with the temperature at which the asymptotic correlation function Eq. (7) begins to cross over from the 1D OZ form at higher temperatures to the low-temperature 2D form.

Figure 5 shows the correlation length for the two-chain ladder at several inter-chain couplings $J_\perp \leq 1$. For $T \approx \Delta(2, J_\perp)$, $\xi(2, J_\perp; T)$ is larger than $\xi_{1D}(T)$ since the ladder system has a higher effective coordination number than the chain. Well below $T = \Delta(2, J_\perp)$, the presence of the nonzero spin gap becomes apparent, and $\xi(2, J_\perp; T \to 0)$ remains finite. With decreasing $J_\perp$, the gap decreases as shown in Fig. 1, and correspondingly, $\xi(2, J_\perp; 0)$ increases from 3.24(5) at $J_\perp = 1$ to 25.6(2) at $J_\perp = 0.15$. In the weak-coupling regime $J_\perp \leq 0.5$, the velocity $c(2, J_\perp) = \Delta(2, J_\perp)\xi(2, J_\perp; 0)$ equals that of the single chain $c_{1D} = \pi/2$ to within the error of our analysis. In this regime the heuristic form

$$\xi^{-1}(2, J_\perp; T) = c_{1D}^{-1}\Delta(2, J_\perp) + \xi_{1D}^{-1}(T)e^{-\Delta(2,J_\perp)/T} \quad (9)$$

describes our correlation length data very well, as shown by the solid lines in Fig. 5. Note that since the spin gap has been determined from measurements of $\chi(T)$, this comparison contains no free parameters.

The temperature dependence of $\xi(2, J_\perp; T)$ in the weak-coupling regime primarily results from that of the single chain, Eq. (8). Apart from logarithmic corrections, the latter is simply $\xi_{1D}(T) \sim T^{-1}$. Equation (9) thus becomes $(\Delta\xi)^{-1} = 2/\pi + A(T/\Delta)e^{-\Delta/T}$, which suggests plotting $\Delta\xi$ versus T/Δ to test for the anticipated scaling for $J_\perp \leq 0.5$. As shown in the inset of Fig. 5, our correlation length data indeed collapse onto a universal curve.

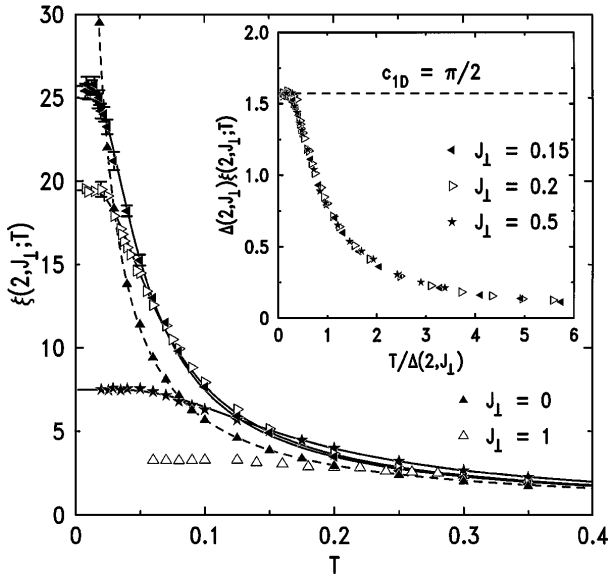

FIG. 5. Correlation length of two antiferromagnetically coupled $S = 1/2$ chains for $J_\perp \leq 1$. The dashed line is Eq. (8), and the solid lines are Eq. (9) with $\Delta(2, J_\perp)$ as obtained from measurements of $\chi(T)$. Inset: Scaling plot of $\Delta(2, J_\perp)\xi(2, J_\perp; T)$ versus $T/\Delta(2, J_\perp)$ for $J_\perp \leq 0.5$.

Over the indicated range the effective value for A is ~ 1.7, compared to the low-temperature value of 2.

For the two-chain ladder, we have established that $\Delta(2, J_\perp \to 0) = 0.41(1)J_\perp$. We can furthermore estimate the weak-coupling behavior for $n_c = 4$. From Fig. 1, it can be inferred that $\Delta(4, J_\perp) \simeq \Delta(2, J_\perp) - 0.35J_\perp$, which leads to $\Delta(4, J_\perp \to 0) = 0.06J_\perp$ as a lower bound. From the lowest $J_\perp$ for $n_c = 4$, we have $\Delta(4, 0.6) = 0.12(1)J_\perp$, which constitutes an upper bound. We thus arrive at the estimate $\Delta(4, J_\perp \to 0) = 0.09(3)J_\perp$.

The trend with increasing n_c of the ladder gap resembles that of the integer-spin single chain as a function of increasing S: For $S = 1$, $\Delta_{S=1} = 0.4105J_\parallel$ is known very accurately [23], while estimates for $S = 2$ range between $\Delta_{S=2} = 0.049(18)J_\parallel$ and $0.085(5)J_\parallel$ [24]. It has recently been argued that the two-chain ladder with antiferromagnetic inter-chain coupling lies in the same phase as the $S = 1$ single chain [25], and that the weak-coupling physics is independent of the sign of $J_\perp$ [11]. Clearly, further numerical and analytical work to establish the correspondence between ladders and chains is necessary.

In summary, our Monte Carlo calculations on spin ladders have provided a number of new results. First, our measured low-temperature correlation function for the weakly coupled two-chain system agrees very well with the predicted theoretical form [11], Eq. (5), which is claimed to be exact. In particular, Eq. (5) captures the crossover in behavior between short and long distances. With increasing temperature the even ladder correlations cross over from the 2D Ornstein-Zernike form to the 1D form of pure exponential decay. Second, for $J_\perp \leq 0.5$ we have discovered that $\Delta(2, J_\perp)\xi(2, J_\perp; T)$ exhibits a rather simple scaling behavior in the variable $T/\Delta(2, J_\perp)$. Third, the structure factor for even n_c exhibits a peak at a temperature well below the corresponding spin gap. Our results for the correlation length and the static structure factor of the isotropically coupled ladders pertain to the experimental systems. For the prototype $S = 1/2$ square-lattice Heisenberg antiferromagnet $Sr_2CuO_2Cl_2$, neutron scattering measurements of the correlation length are in excellent agreement with Monte Carlo simulations and theory [4] as well as high-temperature series expansion [26]. Once sizable single crystals of the ladder systems become available, we intend to extend our neutron scattering work to these interesting systems. We also hope that our Monte Carlo results will motivate future theoretical efforts to predict $C(i, j)$ for general $n_c, J_\perp$, and T.

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[1] H. A. Bethe, Z. Phys. **71**, 205 (1931).
[2] F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983).
[3] See, e.g., I. Affleck, Rev. Math. Phys. **6**, 887 (1994).
[4] M. Greven *et al.*, Z. Phys. B **96**, 465 (1995).
[5] For a review, see E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[6] D. C. Johnston *et al.*, Phys. Rev. B **35**, 219 (1987).
[7] Z. Hiroi *et al.*, J. Solid State Chem. **95**, 230 (1991).
[8] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).
[9] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986); G. Sierra, J. Phys. A **29**, 3299 (1996).
[10] T. Barnes *et al.*, Phys. Rev. B **47**, 3196 (1993).
[11] D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
[12] H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. **70**, 875 (1993).
[13] U.-J. Wiese and H.-P. Ying, Z. Phys. B **93**, 147 (1994).
[14] M. Troyer, H. Tsunetsugu, and D. Würtz, Phys. Rev. B **50**, 13 515 (1994).
[15] M. Reigrotzki, H. Tsunetsugu, and T. M. Rice, J. Phys. C **6**, 9235 (1994).
[16] B. Frischmuth *et al.* (to be published).
[17] N. Hatano and Y. Nishiyama, J. Phys. A **28**, 3911 (1995).
[18] S. R. White and I. Affleck (to be published).
[19] K. Totsuka and M. Suzuki, J. Phys. C **7**, 6079 (1995).
[20] T. T. Wu *et al.*, Phys. Rev. B **13**, 316 (1976).
[21] M. Greven, Ph.D. thesis, Massachusetts Institute of Technology, 1995; see also M. Makivić and H.-Q. Ding, Phys. Rev. B **43**, 3562 (1991).
[22] K. Nomura and M. Yamada, Phys. Rev. B **43**, 8217 (1991).
[23] S. R. White and D. A. Huse, Phys. Rev. B **48**, 3844 (1993); O. Golinelli, Th. Joliceur, and R. Lacace, Phys. Rev. B **50**, 3037 (1994).
[24] S. Yamamoto, Phys. Rev. Lett. **75**, 3348 (1995), and references therein.
[25] S. R. White, Phys. Rev. B **53**, 52 (1996).
[26] N. Elstner *et al.*, Phys. Rev. Lett. **75**, 938 (1995).