

Persistent currents in the Heisenberg chain with a weak link

T. M. R. Byrnes, R. J. Bursill, H.-P. Ecker, and C. J. Hamer*
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia

A. W. Sandvik

Department of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland

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The Heisenberg chain with a weak link is studied as a simple example of a quantum ring with a constriction or defect. The Heisenberg chain is equivalent to a spinless electron gas under a Jordan-Wigner transformation. Using density matrix renormalization group and quantum Monte Carlo methods we calculate the spin/charge stiffness of the model, which determines the strength of the “persistent currents.” The stiffness is found to scale to zero in the weak-link case, in agreement with renormalization group arguments of Eggert and Affleck, and Kane and Fisher.

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I. INTRODUCTION

Technological advances in recent years have allowed the fabrication of electrical and even mechanical devices on the nanometer scale, where individual atoms or electrons can be manipulated. The physics of these devices poses a plethora of fundamental questions through a rich variety of novel quantum effects.¹ This has led to an upsurge of theoretical interest in the physics of “quantum wires,” “quantum dots”, and more general physics at the mesoscopic or nanometer scale.² The effects of electron-electron interactions are typically enhanced in systems of reduced dimensionality, leading to nonperturbative effects such as the breakdown of Fermi liquid behavior in one-dimensional metals, and single-electron charging effects in quasi-zero-dimensional systems (quantum dots). An important milestone in the nascent field of nanomechanics was the experimental discovery that not only the electrical but also the *mechanical* properties of metallic structures on the nanometer scale exhibit apparently universal nonmonotonic quantum corrections,^{3,4} which could be explained theoretically within the framework of a Jellium model.⁵

In the electrical domain, paradigm systems to investigate mesoscopic behavior have long been small ring-shaped or multiply connected devices, where the application of a magnetic flux piercing the device leads to persistent currents. However, the theoretical prediction of these persistent currents, first in superconducting and then in normal conducting materials, has always predated experimental investigation, which has only become feasible in the last decade.⁶ Very recently, with the discovery of a tunable Kondo effect in quantum dots, the persistent currents of multiply connected systems with magnetic quantum dots—Kondo rings for short—have aroused considerable interest.⁷⁻⁹

In this paper we explore a very simple system, which may serve to model a metallic quantum wire ring with a weak junction, or *constriction*. It consists of the standard spin-1/2 Heisenberg antiferromagnetic spin chain, which by a Jordan-Wigner transformation is equivalent to a spinless electron gas in one dimension, where the exchange coupling is weakened at a single link. We use density matrix renormalization

group (DMRG)^{10,11} and quantum Monte Carlo (QMC) methods¹² to obtain numerical results on chains of up to 256 sites, and perform finite-size scaling extrapolations to the bulk limit. We study the spin stiffness, which under the Jordan-Wigner transformation is equivalent to the charge stiffness of the electron gas and is related to the persistent current, as a function of the weak-link coupling. We also study the spin correlations across the weak link.

Eggert and Affleck¹³ have previously studied the Heisenberg chain with an isolated impurity using exact diagonalization and conformal field theory techniques. They find that in renormalization group language a single weak link across the ends of an open chain corresponds to an irrelevant operator, and therefore the open chain is a stable fixed point under such a perturbation. Thus they predict that in the bulk limit a chain with a weak link will behave like an open chain. These findings for a concrete model system are in agreement with the general predictions of Kane and Fisher¹⁴ for the general one-dimensional interacting electron gas, i.e., the Luttinger liquid. An integrable version of the Heisenberg spin chain with defects has also been studied.¹⁵⁻¹⁷ The case of a single defect corresponds to a weak link. However, as opposed to the case discussed here where only one bond is modified, integrability requires a modification of two adjacent bonds and an additional three-spin coupling. Although the defect of this integrable chain is completely transparent to particle scattering, the persistent current is renormalized by the defect strength.

Let us briefly review¹⁸ how the persistent current arises, for the simple case of free electrons. Start from the real-space continuum Hamiltonian

$$H = -\frac{\hbar^2}{2m_e} \sum_{\alpha} \int_0^L dx \psi_{\alpha}^{\dagger}(x) \partial_x^2 \psi_{\alpha}(x) \quad (1)$$

where $\psi_{\alpha}(x)$ is an electron field with spin index $\alpha = \pm 1$, and L is the circumference of the ring. Now thread the ring with a magnetic flux Φ , producing an Aharonov-Bohm effect.¹⁹ The quantum phase

$$\frac{e}{\hbar c} \int_0^L A_\mu d_\mu x = \frac{e}{\hbar c} \Phi \quad (2)$$

can be encoded via a gauge transformation in the twisted boundary conditions

$$\psi_\alpha(L) = e^{i\phi} \psi_\alpha(0), \quad (3)$$

where

$$\phi = 2\pi \frac{\Phi}{\Phi_0}, \quad (4)$$

and $\Phi_0 = hc/e$ is the elementary flux quantum.

When an Aharonov-Bohm field is applied, the Hamiltonian acquires the usual interaction term (we set $\hbar = c = 1$ henceforth)

$$H_{int} = - \int dx A_\mu J^\mu(x). \quad (5)$$

Thus for a constant field $A_1 = \Phi/L$ the corresponding persistent current is given by the Feynman-Hellman theorem:

$$J^1 \equiv I(\Phi) = - \frac{\partial E_0}{\partial \Phi} \quad (6)$$

which can be expanded to

$$I(\Phi) = -D_c \frac{\Phi}{L} + O\left[\left(\frac{\Phi}{L}\right)^2\right] \quad (7)$$

where D_c is the ‘‘charge stiffness.’’ If we *assume* that $I(\Phi)$ is purely linear in Φ (as can be proved for the pure Heisenberg chain²⁰), then the charge stiffness and hence the persistent current can be estimated from the difference in energy between the system with anti-periodic boundary conditions [$E_0^- = E_0(\Phi = \Phi_0/2)$] and periodic boundary conditions [$E_0^+ = E_0(\Phi = 0)$],

$$D_c = \frac{8L}{\Phi_0^2} (E_0^- - E_0^+). \quad (8)$$

The corresponding quantity in the Heisenberg chain is the spin stiffness. In the linear response approximation, it can be shown²¹ that the charge stiffness D_c is equivalent to the Drude weight in the conductivity $\sigma(\omega)$ at frequency ω :

$$\text{Re}[\sigma(\omega)] = \pi D_c \delta(\omega) + \sigma_{reg}(\omega) \quad (9)$$

and

$$\lim_{\omega \rightarrow 0} \omega \text{Im}[\sigma(\omega)] = D_c \quad (10)$$

where $\sigma_{reg}(\omega)$ is regular at $\omega = 0$. A finite value of D_c in the bulk limit indicates a conductor according to the Kohn criterion,²¹ while a zero value indicates an insulator.

In Sec. II of the paper we briefly summarize the DMRG and QMC methods used to calculate this quantity. In Sec. III we present our results, and in Sec. IV our conclusions are summarized.

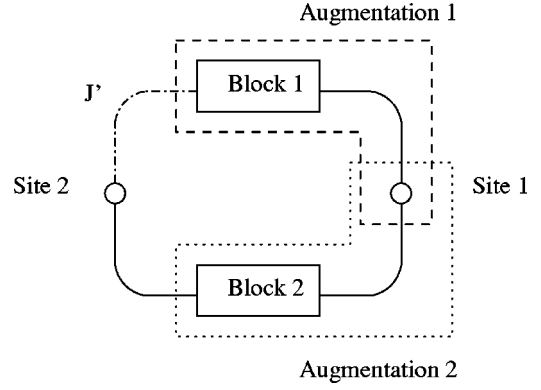


FIG. 1. The augmentation process within one DMRG iteration. Augmentation 1 (Augmentation 2) gives the new Block 1 (Block 2) in the next DMRG iteration.

II. METHOD

We study the spin-1/2 Heisenberg quantum spin chain with a single weak coupling $J' < J$ between two adjacent spins located between sites $i = N$ and $i = 1$. The Hamiltonian is

$$H = J \sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J' \mathbf{S}_N \cdot \mathbf{S}_1. \quad (11)$$

There are a total of N sites in the ring. We study J'/J in the range $[0, 1]$, hence we have either open or periodic boundary conditions (OBC or PBC) at the extremities of this range. We also consider ‘‘twisted’’ antiperiodic boundary conditions in the same range of J'/J ,

$$S_{N+1}^z = S_1^z, S_{N+1}^\pm = -S_1^\pm, \quad (12)$$

which is equivalent to considering a system threaded by a magnetic flux of strength $\pi \hbar c/e$,²² and where we can obtain the charge stiffness D_c according to Eq. (8). The model in these limits is exactly solvable by Bethe ansatz,²³ and hence is often used as a testing ground for various DMRG methods.^{10,24} The quantities that have been calculated using DMRG include the ground-state energy, the singlet and triplet gaps, and correlation functions.

The ‘‘infinite-lattice’’ DMRG method¹⁰ is used here, applied with periodic boundary conditions. The lattice is split into two blocks and two sites as shown in Fig. 1. The weak link is placed between block 1 and site 2. At any time the superblock consists of a system block and an environment block, plus two extra sites. The presence of the weak link destroys the translational invariance normally exploited in usual DMRG schemes, hence we cannot simply make a copy of the density matrix in one block and transfer it to the other block. Therefore in a single DMRG iteration, two density matrices are constructed (one for each block), and the basis set for each block originates from its corresponding density matrix. Each block increases in size by a single site in a single DMRG iteration. We calculate results for lattice sizes $N = 4 - 64$, in steps of two. The quantities calculated here are the ground state energies, and the correlation of the spins

TABLE I. DMRG estimates of the ground-state energy E_0/J and correlation $\langle S_N^z S_1^z \rangle$ for $N=64$ sites at $J'/J=0.5$ as a function of m , the number of states retained per block. A SSE estimate of $E_0/J = -28.2178(3)$ for PBC agrees very well with the DMRG data: here our final DMRG estimate is $-28.21797(1)$. The correlation between spins across the weak link also converges to better than one part in 10^4 . The anti-periodic boundary conditions yield similar levels of accuracy.

m	Periodic		Anti-periodic	
	E_0/J	$\langle S_N^z S_1^z \rangle$	E_0/J	$\langle S_N^z S_1^z \rangle$
96	-28.217 652	-0.060 888	-28.212 779	-0.0560 186
164	-28.217 938	-0.061 194	-28.213 082	-0.0562 742
234	-28.217 964	-0.061 219	-28.213 123	-0.0563 028
342	-28.217 970	-0.061 222	-28.213 132	-0.0563 091

across the weak link. The total number of density matrix eigenstates retained in a block was $m=350$ in the basis truncation procedure.

We also carried out quantum Monte Carlo simulations using the stochastic series expansion (SSE) method.¹² In this case, the spin stiffness can be directly calculated as the second derivative of the energy with respect to the phase, which is given in terms of the fluctuation of the winding number in the simulations.²⁵

III. RESULTS

To estimate the accuracy of the DMRG, we perform convergence tests with m , the number of basis states retained in a block. Table I shows sample results for $J'/J=0.5$ and $N=64$ with both periodic and anti-periodic boundary conditions. We see good convergence with the number of basis states retained: in particular, for the ground-state energy we have convergence to one part in 10^6 . We obtained independent estimates using SSE techniques for the periodic case,

TABLE II. The internal energy and the spin stiffness calculated in SSE simulations for a 256-site chain with $J'/J=1/4$ at different inverse temperatures $\beta=J/T$.

β	E_0/NJ	ρ_s
32	-0.442 11(2)	0.0000(0)
64	-0.442 37(1)	0.0008(1)
128	-0.442 429(9)	0.0088(3)
256	-0.442 443(5)	0.0202(5)
512	-0.442 443(4)	0.0212(4)
1024	-0.442 453(3)	0.0215(2)
2048	-0.442 448(3)	0.0218(2)

which yields $E_0/J = -28.2178(3)$, agreeing perfectly with the DMRG results. The correlations between the spins across the links have a marginally lower accuracy because of round-off error, but even here we have an error in the region of one part in 10^4 .

Since the SSE method is a finite-temperature quantum Monte Carlo method we have to run the simulations at sufficiently low temperature to converge the quantities of interest to their ground state values. In Table II we show the convergence of the energy and the charge stiffness for a 256-site chain. All SSE results discussed below were obtained at inverse temperatures β where the results do not differ, within statistical errors, from results at $\beta/2$.

Ground-state energies were calculated for the periodic and anti-periodic rings, as a function of the weak-link coupling J'/J . Figures 2 and 3 shows DMRG estimates for the quantity $\Delta E_N = [E_0(N; J') - E_0(N; J'=J)]/J$ as a function of J'/J , for several different lattice sizes up to $N=64$. An extrapolation in $1/N$ can be performed to extract the bulk limit for each value of J' by a simple polynomial fit to the data, giving us the extrapolated curve for the periodic and anti-periodic cases. It can be seen that for the periodic case the bulk values are approached from above, while for the anti-

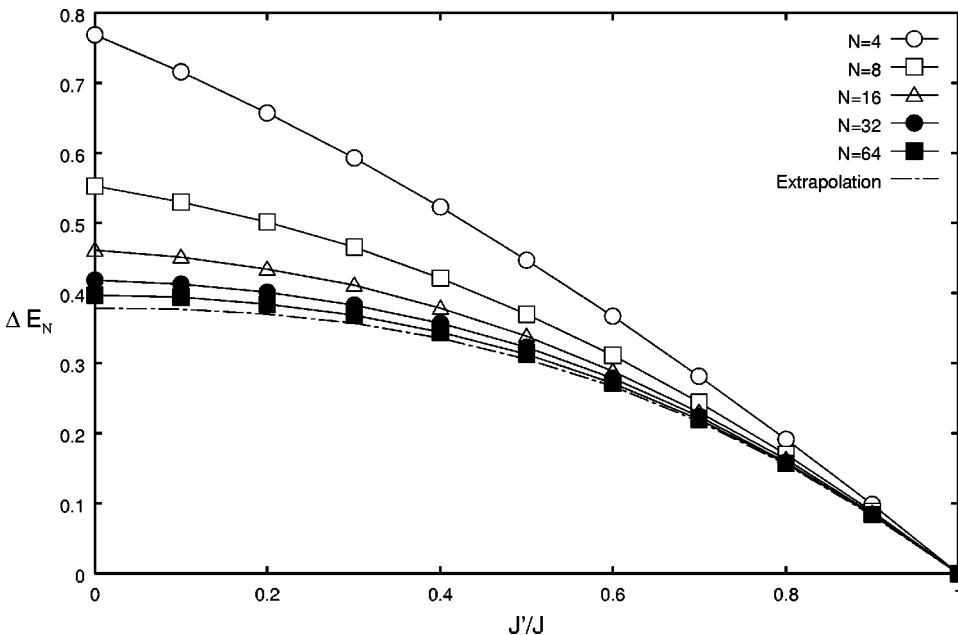


FIG. 2. $\Delta E_N = (E_0(N; J') - E_0(N; J'=J))/J$ as a function of J'/J for the ring with periodic boundary conditions. The data are extrapolated using a simple fit to obtain the bulk limit.

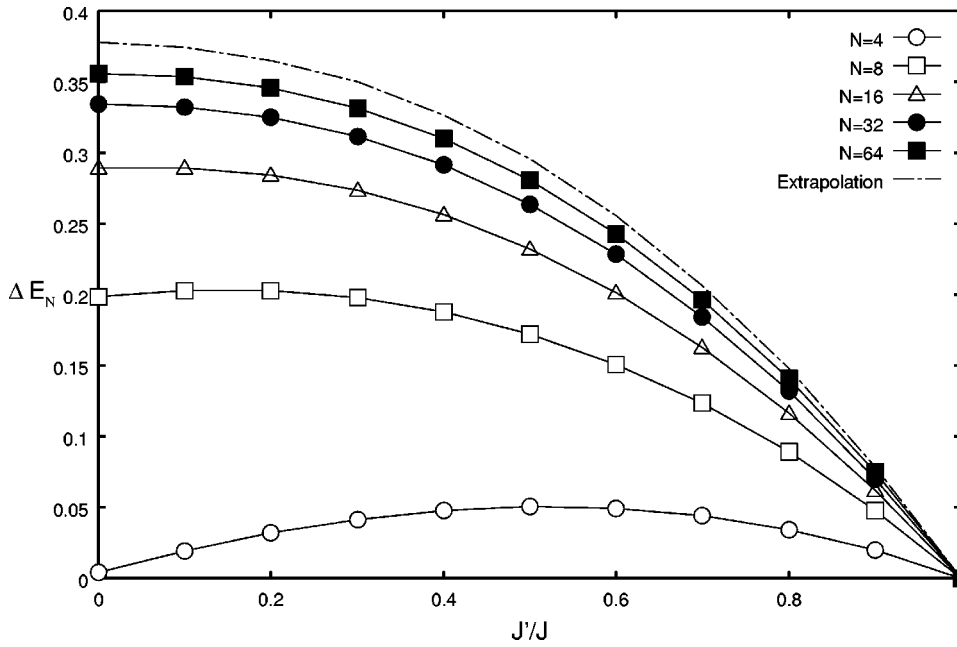


FIG. 3. As for Fig. 2, but with anti-periodic boundary conditions.

periodic case the limit is approached from below.

Putting together both the periodic and anti-periodic results for the energy, we can calculate the spin stiffness factor, given by

$$\rho_s = \frac{2N}{\pi^2 J} [E_0(N; \text{anti-periodic}) - E_0(N; \text{periodic})] \quad (13)$$

The results are shown in Fig. 4. At couplings other than $J'/J=1$ the values trend steadily down towards zero as the lattice size N increases. There is a marked difference in behavior for the isotropic case $J'/J=1$, as the strong curvature towards zero is not apparent. An exact result is available for the $J'/J=1$ case, as obtained by Hamer, Quispel, and Batchelor²⁰ [Equation (3.37) of Ref. 20 with $\gamma=0$],

$$\rho_s = \frac{1}{4}. \quad (14)$$

The apparent discrepancy between the data and this result can be attributed to the presence of logarithmic corrections to the ground-state energy, and hence the stiffness, as shown by Woynarovich and Eckle.²⁶ Such logarithmic effects were observed numerically by Laflorencie, Capponi, and Sørensen,²⁷ who calculated the stiffness for the isotropic model using the Bethe ansatz (see their Fig. 4). Even for a lattice size of 10 000 sites, the stiffness was still above 0.26. A similar effect was noted by Alvarez and Gros,²⁸ who studied the zero momentum limit of the Drude weight (which approaches the spin stiffness), and found it well above 0.25 even for 512 sites.

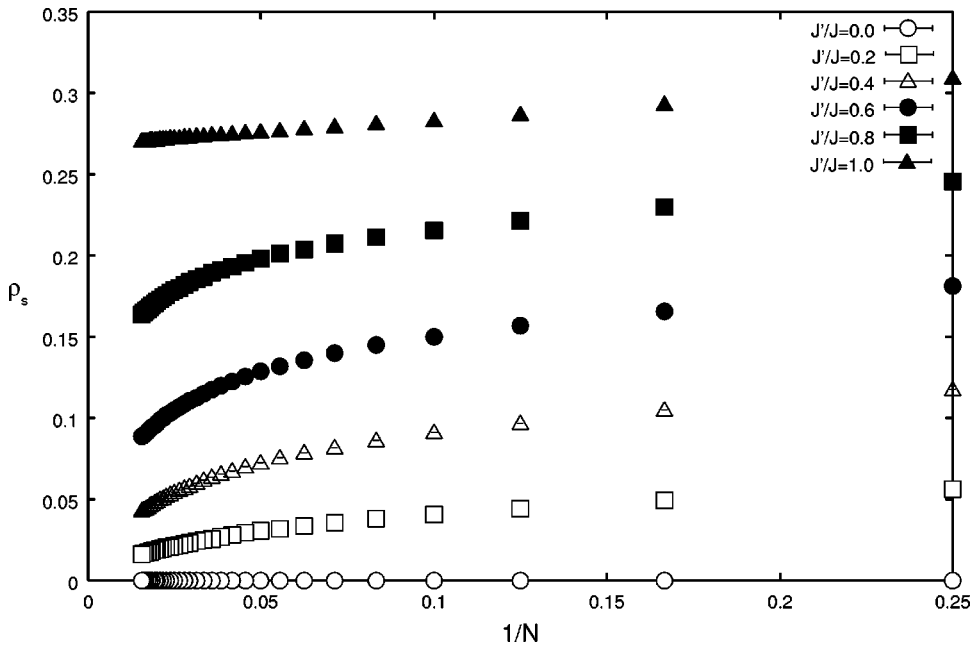


FIG. 4. The stiffness factor ρ_s as a function of $1/N$, for lattice sizes $N=4$ to 64.

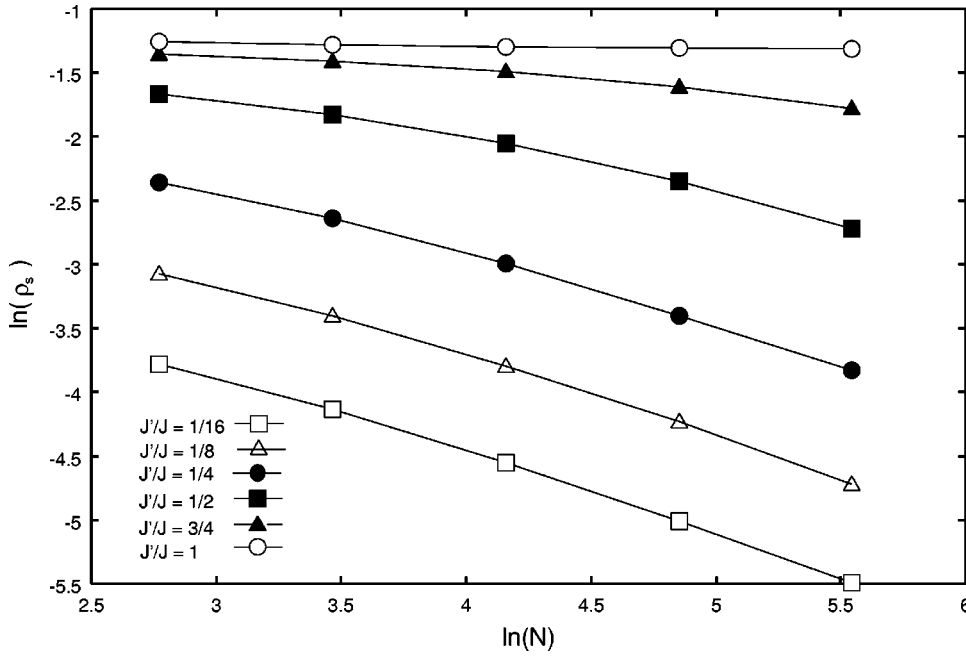


FIG. 5. SSE results for the stiffness factor ρ_s versus lattice sizes ($N=16, 32, 64, 128, 256$).

Using field theoretical methods, Eggert and Affleck¹³ have predicted that a chain with $J' < J$ should be similar to an open chain (i.e., $J'/J=0$). This implies that the spin (charge) stiffness should vanish as the system size $N \rightarrow \infty$. Figure 5 shows SSE results²⁹ for the stiffness versus the system size ($N=16, 32, 64, 128$, and 256) for several values of $J' \leq J$. The results are in accordance with a scaling behavior

$$\rho_N(x) \sim a(x)N^{-\sigma} \quad (15)$$

where $x=J'/J$, and the index $\sigma \approx 2/3$. Figure 6 demonstrates that the data for large N can be well described, in fact, by a simple scaling form

$$\rho_N(x) \sim \frac{2.6x}{(1-x)} N^{-2/3}, \quad N \rightarrow \infty. \quad (16)$$

It is likely, however, that the true asymptotic correction-to-scaling behavior is again being disguised by logarithmic corrections, and that the value $\sigma \approx 2/3$ is only an “effective exponent” valid over the present range of N values, rather than the true asymptotic exponent.

We have also calculated the value of the spin correlation function across the weak link, i.e., $\langle S_N^z S_1^z \rangle$. Figure 7 shows the behavior vs $1/N^2$ for various values of J'/J . It can be seen that the finite-lattice values generally approach a finite value in the bulk limit, as one would expect, except for the special case $J'/J=0$ where the link is open. Theoretical expectations³⁰ are that the correlation function should approach its bulk limit like $1/N^2$, up to logarithmic corrections.

The presence of a finite correlation across the weak link is just what one would naively expect when the weak-link coupling J' is nonzero. On the other hand, it might appear to contradict the previous statement that a chain with a weak link should renormalize to the open chain. The point here is that the weak-link correlation is a *local*, short-distance quan-

tity, not a bulk property. It is integrated out in the early stages of renormalization and then remains fixed, while longer-range correlations will keep renormalizing. It is only bulk properties such as the spin-stiffness which scale to the value of the open chain. Nevertheless, the data of Fig. 7 do show a weak renormalization effect. While the data for $J'/J=1$ remain essentially flat and independent of N , the data for lower values of J'/J exhibit a weak upturn at large N .

IV. CONCLUSIONS

In summary, we have performed a finite-lattice study of the Heisenberg ring with a weak link, using both DMRG and

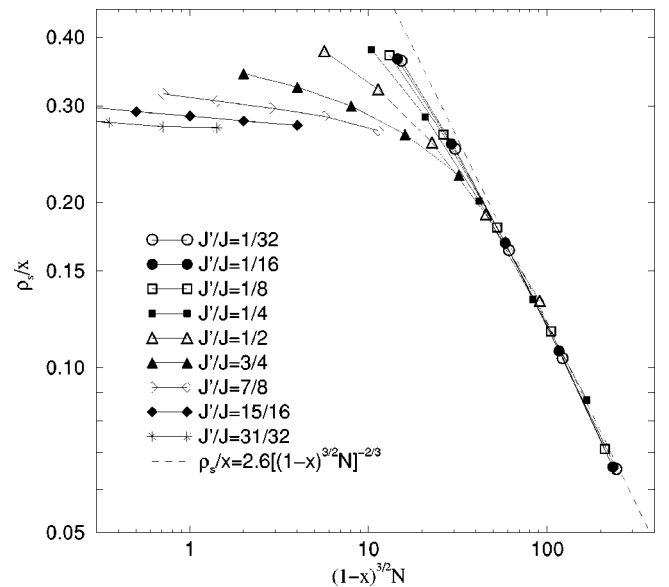


FIG. 6. Scaling plot of ρ_s/x vs $(1-x)^{3/2}N$, where $x=J'/J$. Also shown is the scaling form (16), which agrees with the data for large N .

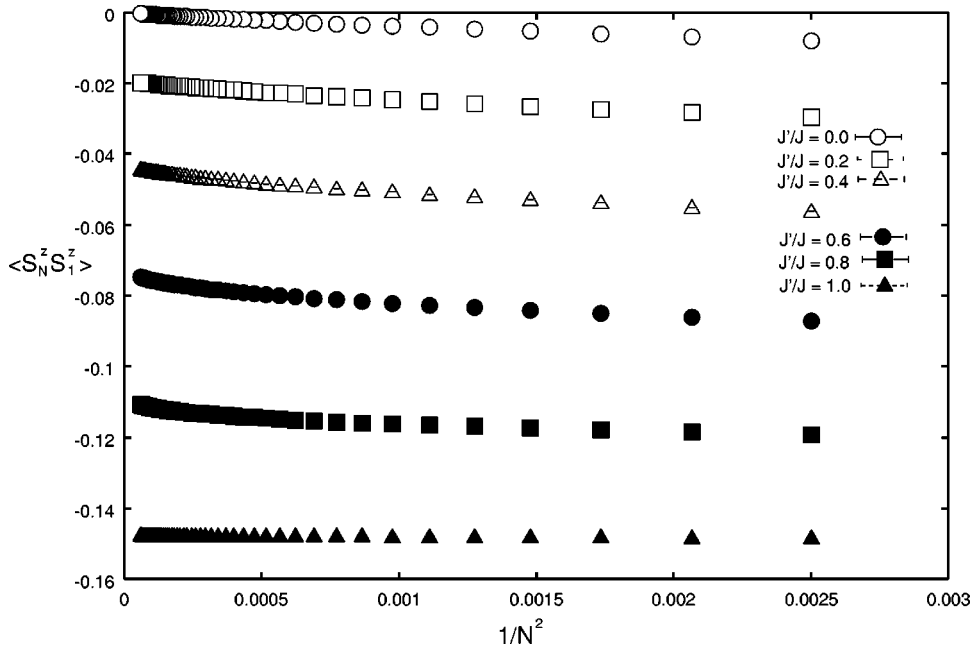


FIG. 7. The correlation $\langle S_N^z S_1^z \rangle$ across the weak link as a function of $1/N^2$.

QMC calculations on rings of up to 256 sites. The spin or charge stiffness has been calculated either directly (QMC), or from the energy difference between the system with anti-periodic boundary conditions and that with periodic boundaries, assuming a quadratic dependence of the energy on the twist parameter ϕ (DMRG).

The stiffness, and hence the persistent current, is found to scale to zero in the bulk limit $N \rightarrow \infty$, for any $J' < J$. This agrees with the renormalization group prediction of Eggert and Affleck,¹³ that the stable fixed point for this system corresponds to an open chain, so that the chain with a weak link will behave like an open chain, as regards its bulk properties.

We have also measured the spin-spin correlation across the weak link. A finite antiferromagnetic correlation remains in the bulk limit, depending on the coupling J' as one would expect. The renormalization group argument does not apply to a local, short-distance property such as this. We note that a similar study of the local spin-spin correlation for the case of an impurity coupled to a Heisenberg chain has been carried out by Zhang, Igarashi, and Fulde.³¹ The asymptotic scaling behavior of these quantities has been disguised to some extent by logarithmic finite-size scaling corrections. Eggert and Affleck¹³ have circumvented this problem by studying a modified model with an extra marginal operator,

but we have not found this necessary for our present purposes.

For the future, it would be of interest to see how the results generalize to more complicated and interesting cases, such as higher spin chains, or real electronic models, such as the Hubbard model or its variant, the so-called $t-J$ model. Another interesting extension of the present study would be to interpret the weak link and hence the modified bond in our model as caused by a mechanical force on a quantum wire. It would be interesting to see what conclusions could be drawn from our simple one-dimensional model for such a scenario.

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*Electronic address: C.Hamer@unsw.edu.au

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