Finite-size study of the ground-state energy, susceptibility, and spin-wave velocity for the Heisenberg antiferromagnet

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The Green's-function Monte Carlo (GFMC) method is used to calculate very accurate ground-state energies of the two-dimensional, spin-$\frac{1}{2}$ Heisenberg antiferromagnet. The computations are performed on $L \times L$ square lattices up to $L = 16$ with varying uniform magnetization, which allows the extraction of the perpendicular susceptibility (χ) and spin-wave velocity (c). These two quantities are the lattice- or cutoff-dependent parameters that allow one to map the long-wavelength properties of the antiferromagnet onto the nonlinear σ model and so are of general interest. Systematic errors present in previous GFMC calculations are addressed and corrected to yield results in excellent agreement with other numerical methods. I find, for the ground-state energy per site, $-0.669\,34(3)$; the susceptibility renormalization factor, $Z_\chi = 0.535(5)$; and the spin-wave velocity renormalization factor, $Z_c = 1.10(3)$. Finite-size effects in the extraction of Z_c and Z_χ are discussed. The value of Z_χ computed here is in agreement with the series-expansion results of Singh and of Zheng, Oitmaa, and Hamer, thereby clearing up a previous inconsistency between the series-expansion and quantum Monte Carlo predictions.

I. INTRODUCTION

Much has been learned about two-dimensional antiferromagnets in recent years. The renewed interest in this area of quantum magnetism has sprung from the desire to understand the undoped phases of the high-T_c superconducting compounds.[1-3] The basic model is that of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet (HAF) on a square lattice, which approximates the undoped high-T_c compounds if the Coulomb repulsion is large.[3] A variety of numerical techniques have demonstrated[4-8,3,9-11] that the ground state of this system has long-range antiferromagnetic order. It had previously been speculated that the order would be destroyed by the strong quantum fluctuations due to the low spin of $\frac{1}{2}$ and low dimensionality.[12] It has been established[13-15] that in an isotropic antiferromagnet the long-wavelength properties can be mapped onto the nonlinear σ model, about which much is known.[1,16,3] This model has (imaginary time) action given by

$$S = \frac{\chi_0 c_0^2}{2} \int_0^\beta d\tau \int_{\mathcal{V}} d\mathbf{x} \left[(\partial_{\mathbf{x}} \mathbf{\Omega})^2 + \frac{1}{c_0^2} (\partial_\tau \mathbf{\Omega})^2 \right] \tag{1}$$

along with the constraint $|\mathbf{\Omega}(\mathbf{x},\tau)| = 1$. The vector $\mathbf{\Omega}$ may be thought of as the local antiferromagnetic order parameter. The two (bare) parameters, χ_0 and c_0, are the perpendicular susceptibility and spin-wave velocity, respectively. If the analogous quantities are computed for a particular isotropic antiferromagnet then the long-wavelength characteristics may be directly mapped to the nonlinear σ model. This type of procedure allows the direct comparison of correlation length measurements[17] (via neutron scattering) in La_2CuO_4 to the predictions of the HAF.[1] The perpendicular (or uniform) susceptibility χ and spin-wave velocity c are related to the spin-stiffness ρ_s by $\rho_s = \chi c^2$, and, so, from the measurement of two of the quantities one may obtain the third (see Sec. III). The quantities χ and c have been computed via long perturbation series expansions about the Ising limit by Singh[8] and by Zheng, Oitmaa, and Hamer,[9] and also via quantum Monte Carlo simulation by Gross, Sanchez-Velasco, and Siggia.[5] The values of χ were found to disagree by about 30%, while the estimated error of each calculation was less than 5%. Since both methods have the possibility of subtle extrapolation complications, it is useful to determine which one is in error. The purpose of this paper is to report reliable Green's-function Monte Carlo (GFMC) calculations of χ and other quantities. The value I find for χ is in agreement with the series expansion results of Refs. 8 and 9. The main improvement needed was to produce sufficiently accurate GFMC $\chi(L)$ data to enable the extrapolation to $L = \infty$ (which amounts to a nearly 30% correction). Since the GFMC extraction of χ requires the finite differencing of energies, the effect of statistical or systematic errors is magnified, and so errors must be carefully estimated. Additionally, I report a very accurate value for the $L = \infty$ ground-state energy per site, E_0/N. The spin-wave velocity is computed as well, along with a discussion of previously ignored finite-size corrections for it. In Sec. II the GFMC algorithm to compute ground-state energies in quantum-spin systems is outlined along with mechanisms for how subtle biases may enter the calculation. In Sec. III the methods to extract χ, c, and E_0/N from the GFMC energies are discussed along with an interpretation of the results.

II. COMPUTATIONAL METHOD

The GFMC algorithm as applied to the HAF is outlined below. Additional details may be found in Refs. 10,

11, and 18. The Hamiltonian of the Heisenberg antiferromagnet is

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2}$$

with [19] $J > 0$. $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ are the components of the vector spin-$\frac{1}{2}$ operator at site i. The sum $\langle ij \rangle$ is over nearest-neighbor pairs on a square lattice consisting of $N = L^2$ sites with periodic boundary conditions.

Letting $\mathcal{S} = (S_1^z, \ldots, S_N^z)$, the Green's-function Monte Carlo algorithm is based on the interpretation of the matrix $K(\mathcal{S}', \mathcal{S}) = \langle \mathcal{S}' | K | \mathcal{S} \rangle$ as a transition probability and of the ground-state wave function $\psi_0(\mathcal{S})$ as the corresponding limit distribution (K is linearly related to H). Importance sampling[20] is crucial to obtaining accurate energies. It is the following similarity transformation of the matrix K in the $\mathcal{S}$ basis:

$$\tilde{K}(\mathcal{S}', \mathcal{S}) = \psi_G(\mathcal{S}') K(\mathcal{S}', \mathcal{S}) / \psi_G(\mathcal{S}) \tag{3}$$

with a known "guiding wave function" $\psi_G(\mathcal{S})$. As $\psi_G \to \psi_0$ one can show the algorithm becomes increasingly efficient. The limit distribution of the kernel $\tilde{K}$ is $\psi_G(\mathcal{S})\psi_0(\mathcal{S})$, and so, the average of the function $E_{loc}(\mathcal{S}) \equiv \langle \mathcal{S} | H | \psi_G \rangle / \psi_G(\mathcal{S})$ over this distribution yields the exact ground-state energy. For ψ_G the nearest-neighbor Gutzwiller wave function of Ref. 11 was used.

The fact that neither K nor $\tilde{K}$ is normalized leads naturally to a *branching* random walk, that is, one with a fluctuating number of random walkers.[10,11,18] The population is kept roughly constant by applying (at iteration or generation n) a multiplicative factor $g(n)$ to the kernel, $\tilde{K}^{(n)} = g(n)\tilde{K}$, to adjust the population up or down to keep it near the desired level. Nearly all GFMC simulations[21] perform a similar type of "population control." The adjustment $g(n)$ introduces a (usually small) bias to the energy because $g(n)$ is correlated with the walk.[22] The bias may be systematically removed by taking larger base populations or by reweighting[23] the measurement (at generation n) with a sufficiently large number k of factors, i.e., $[g(n) \cdots g(n-k)]^{-1}$. There is often a statistically significant bias even with $N_{pop} > 1000$. An example of the convergence with k is shown in Fig. 1. The bias increases with the system size L, evidently because of the smaller effective number of walkers due to longer autocorrelation times, and also increases by the use of a poor guiding function because of the increased branching rate. It is very plausible that the bias due to population control always increases the energy estimate. The structure of the random walk is to replicate a walker when its energy is low and to delete one when its energy is high. So, if there happens to be a tendency to create more walkers (i.e., low energies), then population control may artificially cut it off, and similarly for a tendency to delete walkers (i.e., high energies). Both effects tend to (artificially) raise the energy estimate.

The nonimportance sampled [$\psi_G = 1$ (Ref. 24)] results of Gross, Sanchez-Velasco, and Siggia[5] appear to be biased above the correct values. A possible explanation is as follows. It is known that for the HAF in a given magnetization sector the lowest-lying excited state (total) energies differ from the ground-state energy[25–27] by $E_1 - E_0 = \Delta E \sim 1/L^2$. That is, there is an absolute degeneracy in the ($L \to \infty$) thermodynamic limit. When a fluctuation occurs during the random walk, to project it away requires on the order of

$$\frac{1}{\ln(E_0/E_1)} \sim L^4 \tag{4}$$

generations. Thus, there exists an autocorrelation time[28] in the simulation $\tau \sim L^4$. The number of independent generations is therefore reduced to $\sim N_{gen}/\tau$. Reference 10 has shown that the number of distinct *families* of walkers is nearly inversely proportional to the generation time t, that is, $N_{fam} \propto N_{pop}/t$. During an autocorrelation time of order τ generations a fluctuation can be spread over an entire family. Thus, the number of independent walkers is effectively reduced to $\sim N_{fam} \sim N_{pop}/\tau$. The number of independent "measurements" is therefore roughly

$$N_{ind} \sim N_{gen} N_{pop}/\tau^2 \sim N_{gen} N_{pop}/L^8 . \tag{5}$$

The main point is that N_{ind} decreases rapidly with L, much more so than one might guess. The situation is made worse if poor importance sampling is used, since the increased branching rate makes the rate with which N_{fam} drops off larger. In general, one must be very careful to ensure that N_{ind} is large. The, say, doubling of N_{pop} and extrapolating to $N_{pop} = \infty$ only works if one is in the asymptotic regime.[5]

The results of Trivedi and Ceperley[6] and of Carlson[7] agree with the data I present in Sec. III within the quoted

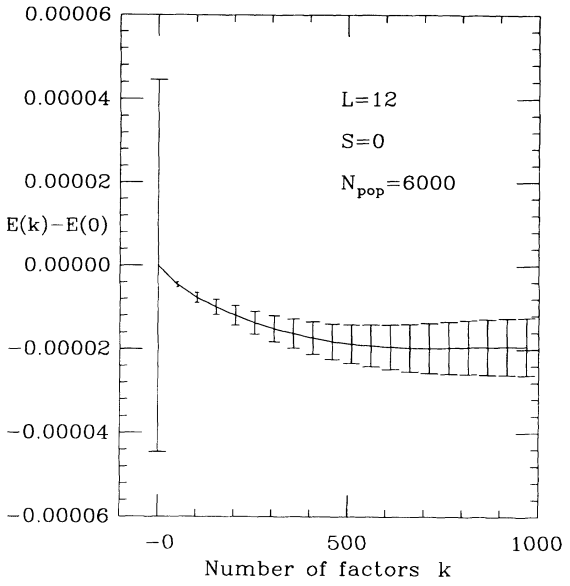

FIG. 1. The removal of the bias due to population control. The ordinate is the difference between the uncorrected energy estimate $E(0)$ and $E(k)$, the one corrected by the removal of k population control factors: $[g(n) \cdots g(n-k)]$. The large error bar at $k = 0$ reflects the statistical error for $E(0)$, while the error bars at $k > 0$ denote the statistical error in the *difference* $E(k) - E(0)$, which is smaller due to correlated sampling.

error bars.[29] However, the fact that most of their data lie above mine suggests that their values may have uncorrected biases on the order of the statistical error. I have attempted to be very careful in addressing biases, but the possibility exists that some may remain in my results as well. Arguments in favor of the quality of my data are (1) I estimate and adjust for the bias introduced by population control, (2) I sample the importance-sampled kernel $\tilde{K}$ *exactly*[11,10] (by rejection) instead of approximately and correcting by additional weights (which increases the amount of branching),[6,7] and (3) my $L \to \infty$ extrapolated ground-state energy is, with high accuracy, inside the error of the series expansion result of Zheng, Oitmaa, and Hamer[9] (see Sec. III).

III. RESULTS AND DISCUSSION

The leading finite-size corrections to the ground-state energy may be written as[25–27]

$$\frac{E(L,S)}{L^2} = \frac{E_0}{L^2} - \frac{1.438c}{L^3} + \frac{1}{2\chi}\frac{S(S+1)}{L^4} + \cdots , \qquad (6)$$

where S is the *total* spin of the system (e.g., singlet $S=0$, triplet $S=1,\ldots$) and is related to the net magnetization by $S=|\sum_i S_i^z|$. The data used to extract the three coefficients in Eq. (6) are listed in Table I. I typically have used $N_{\rm pop}=6000$ and $N_{\rm gen}=10^5$ for $S=0$ and usually a smaller $N_{\rm gen}$ for $S\neq 0$.[30] I first extract E_0/N and c by considering the data with $S=0$. These energies are plotted versus $1/L^3$ in Fig. 2. It is tempting to fit the data to $A+B/L^3$ for $L\geq 6$ as other workers[5–7] have done, since the statistical errors in Table I suggest the relative error in c would be less than 0.3%. The data are too accurate, however, and so cannot be fit with the two parameter function. Using renormalization-group methods,[1] Fisher[26] has predicted that the next-order term (with $S=0$) is proportional to $1/L^5$. This is the same inverse power of L that occurs in the standard spin-wave theory. Fitting the energy data with this extra term yields $E_0/N=-0.669\,34(3)$ and $c=1.55(4)$. The number in the parentheses denotes the error in the last digit. The value for the energy is in agreement with the previously most accurate GFMC result of Carlson[7] [$-0.6692(1)$], and the recent series-expansion calculation of Zheng, Oitmaa, and Hamer[9] [$-0.6694(1)$]. The standard practice is to report c relative to the first-order spin-wave theory result, which in my units ($J=1$) is $c_{\rm SWT}=\sqrt{2}$, thus, $Z_c \equiv c/c_{\rm SWT}=1.10(3)$. It is not clear why this result is outside of the series expansion result by Singh[8] [$Z_c=1.18(2)$]. See, however, the discussion in the following paragraph on the possibility of different fitting forms.[31] For comparison, the second-order spin-wave theory has $Z_c=1.158$.

As mentioned above, the $6\leq L\leq 16$ energies in Table I. are not fit by a straight line in $1/L^3$. Indeed, the data suggest a 5–10% increase of slope [that is to say, an increase in $c(L)\propto \partial E/\partial(L^{-3})$] in going from $L=10$ to ∞.

TABLE I. Green's-function Monte Carlo results for the ground-state energy per site for different lattice sizes $N=L^2$ and with varying total spin S. The number in the parentheses is the error in the last digit(s). For example, $-0.661\,304(12)$ denotes -0.661304 ± 0.000012.

	S	Energy
$L=6$	0	$-0.678\,871(8)$
	1	$-0.670\,878(10)$
	2	$-0.655\,092(9)$
	3	$-0.631\,591(10)$
$L=8$	0	$-0.673\,486(14)$
	2	$-0.665\,325(8)$
	3	$-0.657\,258(10)$
	4	$-0.646\,609(9)$
	5	$-0.633\,447(12)$
$L=10$	0	$-0.671\,492(27)$
	3	$-0.664\,533(13)$
	4	$-0.659\,873(13)$
	6	$-0.647\,392(11)$
	8	$-0.630\,642(18)$
$L=12$	0	$-0.670\,581(49)$
	5	$-0.661\,934(9)$
	8	$-0.650\,041(16)$
	10	$-0.639\,518(5)$
$L=16$	0	$-0.669\,872(28)$
	9	$-0.661\,304(12)$
	13	$-0.652\,809(5)$
	17	$-0.641\,592(10)$
	21	$-0.627\,968(30)$

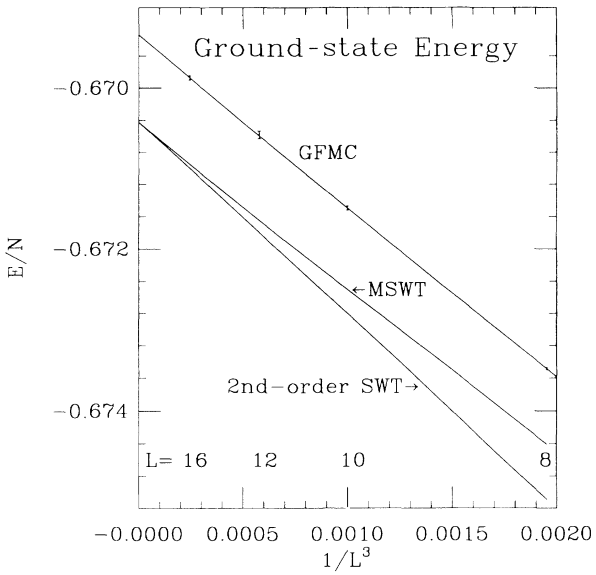

FIG. 2. Singlet ground-state energy per site E/N vs $1/L^3$. GFMC denotes the Green's-function Monte Carlo results of the present work. The curve is the fit involving terms up to $1/L^5$ described in text. The intercept at $L=\infty$ is $E/N=-0.669\,34(3)$. MSWT are the results of the modified spin-wave theory described in Ref. 34. The standard second-order spin-wave predictons are also displayed. (See Ref. 3 for a discussion.)

Thus, the Monte Carlo calculations of Z_c with no $1/L^5$ fitting term may have a 10% systematic error, since values of L less than 10 are used to extract Z_c. The modified spin-wave theory (MSWT) of Arovas and Auerbach,[32] Takahashi,[33] and Tang and co-workers[34] is a surprisingly accurate theory for the spin-correlation functions and energies on *finite* lattices. As $L\to\infty$ the theory reproduces the second-order spin-wave predictions. The second-order spin-wave and MSWT energies are plotted in Fig. 2 with the simulation results. Although it is difficult to see, the MSWT appears to reproduce the slight upward curvature in energy versus $1/L^3$. This is not surprising, since the theory describes small lattices rather accurately. Like the GFMC data, the MSWT has about a 10% change in $c(L)$ from $L=10$ to ∞. Numerically I find that the MSWT has $1/L^4$ as its subleading finite-size correction rather than $1/L^5$ as predicted by Fisher. Fitting the GFMC data to $A+B/L^3+C/L^4$ gives $Z_c=1.15(3)$ and an E_0/N changed only slightly from the one quoted above. This latter value of Z_c appears to be in closer agreement with the other numerical calculations.[3] It should be noted that the MSWT was able to predict terms in the low-temperature expansion of the one-dimensional Heisenberg ferromagnet[35] that are missing from the ordinary spin-wave theory prediction. Unfortunately, GFMC calculations of much higher accuracy and on larger lattices would be required to distinguish between $1/L^4$ and $1/L^5$ subleading corrections.

I now turn to the calculation of the perpendicular susceptibility χ. From Eq. (6) one can define an effective susceptibility $\chi_{\rm eff}(L,S)$ through

$$\frac{1}{2\chi_{\rm eff}(L,S)}\equiv\frac{[E(L,S)-E(L,0)]L^2}{S(S+1)}=\frac{1}{2\chi}+\cdots . \tag{7}$$

Using the GFMC data, one finds that there is a substantial S dependence[36] in $\chi_{\rm eff}(L,S)$ (L fixed) and so once again we need a higher-order term in Eq. (6). Fisher[26] has shown for the infinite system that

$$\varepsilon(H)=\varepsilon_0-\frac{\chi}{2}H^2-\frac{1}{12\pi c^2}|H|^3+\cdots , \tag{8}$$

where here H is an applied uniform field and ε is the ground-state energy per site. If M is the magnetization per site that H couples to, then the standard Legendre transformation, $\varepsilon(H)=\varepsilon(M)-MH$, yields

$$\varepsilon(M)=\varepsilon_0+\frac{1}{2\chi}M^2-\frac{1}{12\pi c^2}\left[\frac{|M|}{\chi}\right]^3+\cdots . \tag{9}$$

To estimate finite-size corrections, one makes the replacement $M^2\to S(S+1)/N^2\equiv x$, which implies

$$\varepsilon(x)=\varepsilon_0+\frac{1}{2\chi}x-\frac{1}{12\pi c^2\chi^3}|x|^{3/2}+\cdots . \tag{10}$$

The above suggests that $1/2\chi_{\rm eff}\ \{\equiv[\varepsilon(x)-\varepsilon_0]/x\}$ should have a $\sqrt{x}$ correction term. Indeed, the GFMC data fit this form quite well: both the *sign* and approximate size of the $\sqrt{x}$ correction agree with that implied in Eq. (10). The above form has been used to extrapolate to $x=0$. The resulting values of $1/2\chi_{\rm eff}(L)$ are plotted vs $1/L$ in Fig. 3. By exploiting certain universal amplitude ratios, Fisher[26] has noted that there should be a sizable $1/L$ finite-size contribution in $\chi(L)$, and it should be comparable to the observed correction in the staggered magnetization $M^\dagger(L)$.[4,37,3,11] For example, $M^\dagger(L)$ has a reduction of 33% in going from $L=6$ to ∞, and the $\chi(L)$ computed here has a 31% reduction for the same variation of L. To extrapolate to $L=\infty$, I fit $1/2\chi_{\rm eff}$ to $A+B/L+C/L^2$. The result is $\chi=0.0669(7)$ or $Z_\chi=\chi/\chi_{\rm SWT}=0.535(5)$. The value is in agreement with the series expansion calculations of Singh[8] [$Z_\chi=0.52(3)$] and of Zheng *et al.*[9] [$Z_\chi=0.527(8)$], and is substantially outside of the quantum Monte Carlo estimate by Gross, Sanchez-Velasco, and Siggia [$Z_\chi=0.71(4)$] and the second-order spin-wave result ($Z_\chi=0.448$).

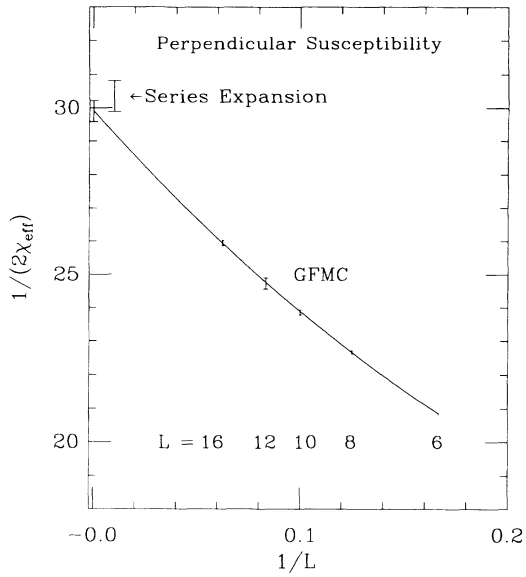

FIG. 3. Extrapolation of the GFMC inverse perpendicular susceptibility $1/2\chi$ to the thermodynamic limit. Solid line is the fit described in text. Intercept is 29.9(3). Units are those of Ref. 5 ($J=4$) that found 22.5(13). The series expansion result is that of Ref. 9, and is displaced from zero for clarity.

In summary, I have reported accurate GFMC ground-state energy calculations on the spin-$\frac{1}{2}$ HAF along with a discussion on how systematic biases may be avoided. From these data I have estimated the $L\to\infty$ limits of the ground-state energy per site E_0/N, and the spin-wave velocity c, and the perpendicular susceptibility χ. For these quantities, both leading *and* subleading finite-size corrections are required to fit the data. The author knows of no other quantum Monte Carlo calculations that have considered these terms. In spite of the increased error that accompanies additional fitting parameters, this study has produced the most accurate values to date for E_0/N and χ. Most importantly, the GFMC result for χ now agrees with the series expansion calculations in Refs. 8 and 9. The value for c still appears to lie outside of the best estimate,[8] and so more effort is required to clear up the

$\sim 8\%$ discrepancy. The prospect of directly measuring the spin stiffness $\rho_s (Z_{\rho_s} = Z_\chi Z_c^2)$ via GFMC is currently being investigated and may provide useful information on the true value of c.

Accurate values for E_0/N, Z_c, and Z_χ are important because, through the nonlinear σ model, they allow a direct comparison with experimental correlation length measurements and also because they provide useful "benchmark" data against which variational and other analytical methods may be tested. Third-order spin-wave calculations should be accomplished soon,[38] and the comparison of them to the exact results should prove illuminating. This work has shown that the GFMC algorithm can be used to compute energies in spin systems to within one part in 10^4–10^5 for lattices consisting of several hundred sites. Hopefully, this powerful tool will find many applications in the field of quantum magnetism.

ACKNOWLEDGMENTS

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[30] Note that the GFMC autocorrelation should go as $\tau = \tau(L,S) \sim L^4/(S+1)$, and so it is unwise to expect the bias due to population control to cancel out in finite differences with respect to S.

[31] Also, using the more accurate result for Z_χ from Zheng, Oitmaa, and Hamer in Ref. 9 and Singh's (Ref. 8) result for the spin stiffness factor $Z_{\rho_s} = 0.72(4)$ suggests that Z_c $[\equiv (Z_{\rho_s}/Z_\chi)^{1/2}] = 1.169(33)$, which nearly overlaps with the present result $Z_c = 1.10(3)$. This estimate is computed in exactly the same manner as in Ref. 8 except that the value of Z_χ from Ref. 9 is used instead of that of Ref. 8.

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