Numerical study of a two-dimensional quantum antiferromagnet with random ferromagnetic bonds

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A Monte Carlo method for finite-temperature studies of the two-dimensional quantum Heisenberg antiferromagnet with random ferromagnetic bonds is presented. The scheme is based on an approximation which allows for an analytic summation over the realizations of the randomness, thereby significantly alleviating the "sign problem" for this frustrated spin system. The approximation is shown to be very accurate for ferromagnetic bond concentrations of up to 10%. The effects of a low concentration of ferromagnetic bonds on the antiferromagnetism are discussed.

Monte Carlo studies of frustrated quantum spin systems are difficult since positive definite weight functions cannot be constructed in general (the so-called "sign problem").[1,2] For random models, on the other hand, averaging over a large number of realizations of the randomness is necessary, which considerably increases the computational effort over what is required for nonrandom systems. Both the above difficulties are present for the antiferromagnetic Heisenberg model with random ferromagnetic bonds. The two-dimensional (2D) version of this model is of current interest as a possible model of the copper-oxygen sheets of lightly doped, but still insulating high-T_c superconductor materials. The idea, stressed by Aharony *et al.*,[3] is that in the doped insulating phase, the holes introduced into the Cu-O sheets are localized at individual oxygen sites. The coupling between the copper and oxygen spins results in an effective *ferromagnetic* coupling between the copper spins adjacent to an oxygen spin. Due to the computational problems mentioned above, this picture has not yet been tested by direct numerical calculations of experimentally measurable quantities of the proposed model Hamiltonian.

Previous numerical work on random quantum spin systems has been largely limited to 1D systems[4] and nonfrustrated 2D models.[5] Quantum Monte Carlo simulations of random systems with frustration have been carried out in cases where the sign problem is not present, such as the Ising spin glass in a transverse field.[6] For models with random long-range interactions, recent progress has been made using field-theoretic methods.[7]

In this paper a Monte Carlo method for finite-temperature studies of the 2D Heisenberg model with mixed antiferromagnetic and ferromagnetic nearest-neighbor couplings of equal strengths is presented. The scheme employs an approximation which corresponds to an annealing of the quenched disorder. This approximation is argued to be very accurate in the regime of interest for the high-T_c cuprates; a concentration of ferromagnetic bonds of less than 10%. The summation over all realizations of the annealed randomness can be carried out analytically for each Monte Carlo configuration, thereby significantly alleviating the sign problem. Furthermore, in a single simulation, calculations can be carried out for several concentrations of ferromagnetic bonds with essentially no additional computational cost.

Below, the method is described and tested for small systems. Results are presented for the effect of an increasing concentration of ferromagnetic bonds on the staggered structure factor and the uniform susceptibility.

The model is defined by the Hamiltonian

$$\hat{H} = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $\langle i,j \rangle$ is a pair of nearest-neighbor sites on a square lattice, and $\mathbf{S}_i$ is a spin-$\frac{1}{2}$ operator at site i. The coupling constants J_{ij} are all of equal strength J, but their signs are random, with a probability ρ for $-J$ (ferromagnetic) and $1-\rho$ for $+J$ (antiferromagnetic). In its current formulation the method to be presented does not allow for different ferromagnetic and antiferromagnetic coupling strengths. The random $\pm J$ model should, however, exhibit the general features associated with the presence of a low concentration of frustrating bonds.

The computational scheme will be discussed in the context of a generalization of Handscomb's quantum Monte Carlo method,[8] but the same idea should be applicable to "world-line" methods[9] as well. Consider the expectation value of an operator $\hat{A}$ at inverse temperature $\beta = 1/k_B T$:

$$\langle \hat{A} \rangle = \frac{1}{Z} \mathrm{Tr}\{\hat{A} e^{-\beta \hat{H}}\}, \quad Z = \mathrm{Tr}\{e^{-\beta \hat{H}}\}. \tag{2}$$

The starting point for the generalization of Handscomb's method is to Taylor expand $e^{-\beta \hat{H}}$ and to write the traces in (2) as sums over diagonal matrix elements in a suitably chosen basis $\{|\alpha\rangle\}$, giving for the partition function

$$Z = \sum_{n=0}^{\infty} \sum_{\alpha} \frac{(-\beta)^n}{n!} \langle \alpha | \hat{H}^n | \alpha \rangle. \tag{3}$$

For the Heisenberg model, the basis $\{|S_1^z, \ldots, S_N^z\rangle\}$, $S_i^z \in \{\uparrow, \downarrow\}$, is chosen, and the Hamiltonian (1) is written as

$$\hat{H} = -\frac{J}{2}\sum_{b=1}^{N_b}\sigma_b\Big[H_{1,b} - H_{2,b}\Big] + N_b(1-2\rho)J/4, \quad (4)$$

where

$$\begin{aligned}\hat{H}_{1,b} &= 2(\tfrac{1}{4} - S^z_{s1(b)}S^z_{s2(b)}) \ , \\ \hat{H}_{2,b} &= S^+_{s1(b)}S^-_{s2(b)} + S^-_{s1(b)}S^+_{s2(b)}. \end{aligned} \quad (5)$$

Here $s1(b)$ and $s2(b)$ are the sites connected by bond b, $N_b = 2L^2$ is the number of bonds of the lattice, and σ_b is -1 if b is a ferromagnetic bond and $+1$ otherwise. The partition function can now be written as

$$Z = \sum_{n=0}^{\infty}\sum_{S_n}\sum_{\alpha}\frac{(-1)^{n_F}(\beta J/2)^n}{n!}\Big\langle\alpha\Big|\prod_{i=1}^{n}H_{a_i,b_i}\Big|\alpha\Big\rangle, \quad (6)$$

where S_n denotes a sequence of n index pairs,

$$S_n = \binom{a_1}{b_1}_1\binom{a_2}{b_2}_2\cdots\binom{a_n}{b_n}_n, \quad (7)$$

with $a_i \in \{1,2\}$, $b_i \in \{1,\ldots,N_b\}$ referring to an operator $\hat{H}_{a,b}$. The matrix element in (6) is equal to 0 or 1, and the sign of a given term is determined only by the number n_F of operators $\hat{H}_{a,b}$ with b being one of the ferromagnetic bonds. This sign rule is valid for a bipartite lattice, in which case an operator string contributing to Z must flip each spin in $|\alpha\rangle$ an even number of times, and therefore the total number of operators $\hat{H}_{2,b}$ must be even. Note that the only dependence on the realization of the randomness in (6) is in the number n_F. This is crucial in what follows.

The actual Monte Carlo scheme has been described elsewhere,[8] and will not be discussed here. It suffices to note that, as has been shown above, for a given realization R of the $\pm J$ bonds on the lattice, an operator expectation value can be written as

$$\langle\hat{A}\rangle_R = \frac{\sum_C W_C A_C S_C(R)}{\sum_C W_C S_C(R)}, \quad (8)$$

where W_C is a positive definite weight for the configuration C (C here belongs to the space $\{\alpha, S_n, n = 0,1,2,\ldots\}$ of states and index sequences), $S_C(R) = (-1)^{n_F(R)}$ is a sign which depends on the realization R as well as C, and A_C is a function measuring the operator $\hat{A}$ (the construction of A_C for various types of operators is discussed in detail in Ref. 8). Here only operators without explicit dependence on the particular realization of the randomness will be considered, e.g., bulk susceptibilities and magnetic structure factors.

In a Monte Carlo simulation the configurations C are generated using W_C as a relative probability distribution, and the quantities $S_C(R)$ and $A_C S_C(R)$ are measured with regular intervals. The expectation value of $\hat{A}$ is then given by[9]

$$\langle\hat{A}\rangle_R = \frac{\langle A_C S_C(R)\rangle}{\langle S_C(R)\rangle}, \quad (9)$$

and the average over the realizations of the randomness is

$$\langle\langle\hat{A}\rangle\rangle = \frac{1}{N_R}\sum_R\frac{\langle A_C S_C(R)\rangle}{\langle S_C(R)\rangle}, \quad (10)$$

where N_R is the number of realizations. If $\langle S_C(R)\rangle \ll 1$, accurate determinations of $\langle S_C(R)\rangle$ and $\langle A_C S_C(R)\rangle$ become very time consuming. Since $\langle S_C(R)\rangle$ in most cases approaches zero exponentially as the temperature is lowered, the sign problem is a severe limitation of the quantum Monte Carlo technique for models where one cannot construct (e.g., using symmetries) a weight function with a sign identically equal to one.[2]

Since the weight W_C does not depend on the realization of the randomness, an estimate of $\langle\langle\hat{A}\rangle\rangle$ can be obtained by carrying out the measurements of $A_C S_C(R)$ and $S_C(R)$ on a set of pregenerated realizations in a single Monte Carlo simulation. Hence, the randomness averaging does not pose a problem. However, this by itself does not alleviate the sign problem, as the evaluation of the individual terms of (10) still becomes unstable when $S_C(R) \ll 1$. The approximation introduced next will be shown to significantly reduce this sign problem.

Consider the expectation values $\langle A_C S_C(R)\rangle$ and $\langle S_C(R)\rangle$ averaged over the randomness:

$$\begin{aligned}\langle\langle S_C\rangle\rangle &= \frac{1}{N_R}\sum_R\langle S_C(R)\rangle \ , \\ \langle\langle A_C S_C\rangle\rangle &= \frac{1}{N_R}\sum_R\langle A_C S_C(R)\rangle \ . \end{aligned} \quad (11)$$

The realization-dependent averages can be written in terms of their deviations from the respective realization-averaged quantities as

$$\begin{aligned}\langle A_C S_C(R)\rangle &= \langle\langle A_C S_C\rangle\rangle + \Delta_{AS}(R) \ , \\ \langle S_C(R)\rangle &= \langle\langle S_C\rangle\rangle + \Delta_S(R). \end{aligned} \quad (12)$$

A realization-averaged expectation value can then be written as

$$\langle\langle\hat{A}\rangle\rangle = \frac{\langle\langle A_C S_C\rangle\rangle}{\langle\langle S_C\rangle\rangle} + \mathcal{O}(\Delta^2), \quad (13)$$

where $\mathcal{O}(\Delta^2)$ denotes terms of order $\Delta_{AS}(R)\Delta_S(R)$ and $(\Delta_S(R))^2$. [Note that (13) would be exact if $\Delta_S(R)$ would be zero for all R, even with $\Delta_{AS}(R) \neq 0$.] If the concentration of ferromagnetic bonds is low, the approximation (13) can be expected to be a good one, since the main contribution to $\langle\langle\hat{A}\rangle\rangle$ is from realizations where the ferromagnetic bonds are far apart from each other. The signs $\langle S_C(R)\rangle$ should then typically be insensitive to variations in R. Note, however, that the approximation *does* contain collective impurity effects, as the averages in (13) depend in a nontrivial manner on the number of ferromagnetic bonds present.

Under the above approximation, the averages over the Monte Carlo configurations and the realizations of the randomness have been put on an equal footing. This corresponds to going from quenched to annealed disor-

der. The computational advantage is that the averaging over the randomness can be performed *analytically* for each Monte Carlo configuration, which in effect means that each Monte Carlo measurement step corresponds to measuring on a very large number N_R of configurations, which for a fixed number N_f of ferromagnetic bonds is given by

$$N_R = \binom{N_b}{N_f}. \tag{14}$$

One might hope that this averaging enables a stable evaluation of the expectation values $\langle\langle S_C\rangle\rangle$ and $\langle\langle A_C S_C\rangle\rangle$ far beyond the point where estimates of $\langle A_C S_C(R)\rangle$ and $\langle S_C(R)\rangle$ become too noisy.

Denoting by $F(R)$ the set of ferromagnetic bonds in the realization R, the sign of a Monte Carlo configuration can be written as

$$S_C(R) = \prod_{b\in F(R)} (-1)^{n_b} = \prod_{b\in F(R)} s_C(b), \tag{15}$$

where n_b is the number of operators acting on bond b, i.e., the number of index pairs $\binom{a_i}{b_i}$ with $b_i = b$ in S_n. Hence the sign is a product of "local signs" $s_C(b)$, with $s_C(b)$ being positive or negative depending on if n_b is even or odd. Note that the local signs depend only on the Monte Carlo configuration C, and the full sign $S_C(R)$ is calculated using only the local signs of the ferromagnetic bonds of R. Denoting the total number of local minus signs by n_- and the total number of local plus signs by $n_+ = N_b - n_-$, the randomness averaged sign $\Sigma_C = \frac{1}{N_R}\sum_R S_C(R)$ of a Monte Carlo configuration is given by

$$\Sigma_C = \frac{1}{N_R}\sum_{f=0}^{N_f}(-1)^f \binom{n_-}{f}\binom{n_+}{N_f - f}. \tag{16}$$

The (approximate) Monte Carlo estimate (13) for the disorder averaged $\langle\hat{A}\rangle$ can now be written as

$$\langle\langle\hat{A}\rangle\rangle = \frac{\langle A_C\Sigma_C\rangle}{\langle\Sigma_C\rangle}, \tag{17}$$

where all effects of the randomness is contained in Σ_C, which can be easily calculated for each Monte Carlo configuration.[10]

Next it will be demonstrated that this estimate of $\langle\langle\hat{A}\rangle\rangle$ is indeed considerably less noisy than (13), and that the approximation involved is very good, at least when the concentration of ferromagnetic bonds is low. Results will be shown for the staggered structure factor

$$S(\pi,\pi) = \frac{1}{L^2}\sum_{j,k} e^{i\pi\cdot(\mathbf{r}_k - \mathbf{r}_j)}\langle\langle S_j^z S_k^z\rangle\rangle \tag{18}$$

and the uniform susceptibility

$$\chi(0,0) = \frac{1}{L^2}\sum_{j,k}\int_0^\beta d\tau\langle\langle S_j^z(\tau)S_k^z(0)\rangle\rangle. \tag{19}$$

In order to test the accuracy of the "annealed" approximation, simulations of $L\times L$ systems with $L = 4$ and 8 were carried out, and $S(\pi,\pi)$ and $\chi(0,0)$ were calculated using both (10) and (17) [with (10), the averaging over R was done for using several hundred randomly generated realizations]. Figure 1 shows results for $L = 4$ at temperatures $T/J = 0.4$, 0.6, and 0.8. The maximum ferromagnetic bond concentration for which the averages can be evaluated decreases rapidly as the temperature is lowered. As expected, the approximate averages are easier to obtain than the exact ones. Perhaps surprisingly, no deviations of the approximate averages from the exact ones can be seen within statistical errors, even for rather high ρ. The antiferromagnetism is strongly suppressed by the disorder; the staggered structure factor decreases with ρ and the uniform susceptibility is enhanced. The effect becomes stronger as the temperature is decreased. Figure 2 shows similar results for 8×8 systems. Here the suppression of the antiferromagnetism is even stronger. Again, no differences between the approximate and exact results can be seen up to the maximum ρ for which they can both be reliably calculated. One might expect the errors of the annealed approximation to become larger at lower temperatures, where comparisons are difficult due to the sign problem.

Figure 3 shows the average sign versus the number of

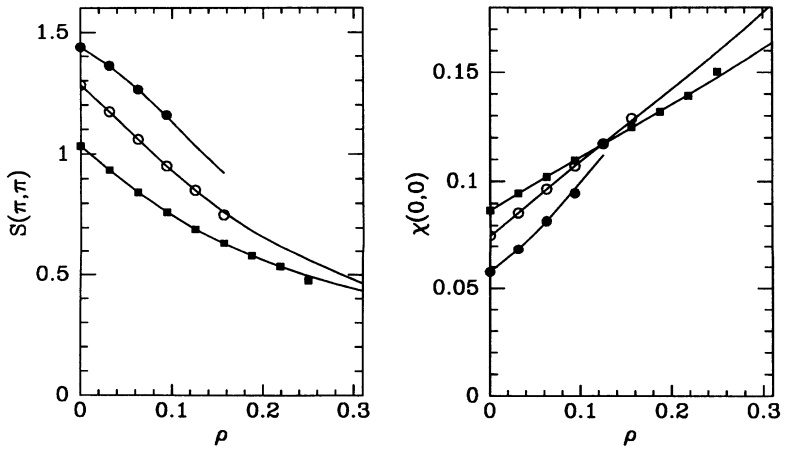

FIG. 1. The staggered structure factor and the uniform susceptibility vs the ferromagnetic bond concentration for $L = 4$ at three different temperatures. Results obtained using (10) are shown as solid squares ($T/J = 0.8$), open circles ($T/J = 0.6$), and solid circles ($T/J = 0.4$). The solid curves are drawn through points obtained using the "annealed" approximation (17).

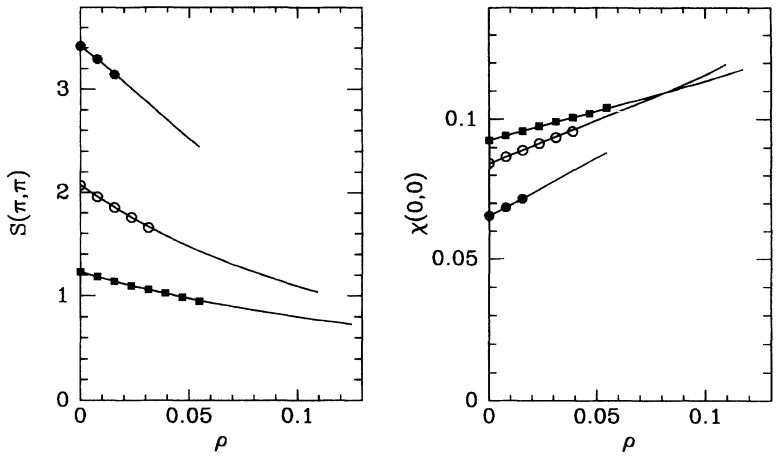

FIG. 2. Same as Fig. 1 for systems of size 8×8.

ferromagnetic bonds for $L = 4$ and $L = 8$ at $T/J = 0.4$, 0.6, and 0.8. There is very little size dependence, confirming that the average sign at a given temperature depends essentially only on the number of ferromagnetic bonds present. Note that $\langle \Sigma_C \rangle$ can be accurately evaluated for the larger system even when it becomes extremely small.[10] Using the exact expression (10) is not feasible if $\langle S_C(R) \rangle$ becomes smaller than $\approx 10^{-3}$. This limits the maximum number of ferromagnetic bonds that can be studied. An accurate calculation of $\langle \Sigma_C \rangle$, on the other hand, is possible up to some maximum ρ, which is essentially independent of the system size. The evaluation of the expression (17) still becomes more difficult as the system size increases for operators such as the staggered structure factor, for which the autocorrelation time grows with the system size and fluctuations in $\langle A_C \Sigma_C \rangle$ become problematic.

The model (1) has antiferromagnetic long-range order at $T = 0$ for $\rho \to 0$ and ferromagnetic order for $\rho \to 1$. At intermediate ρ there is presumably a spin-glass phase. An important open question is the critical concentration of ferromagnetic bonds needed to destroy the antiferromagnetism. In principle finite-size scaling of the staggered structure factor can answer this question, which however is beyond the scope of this paper. Here some initial results for the effect of an increasing fraction of ferromagnetic bonds on systems of size 10×10 are presented.

In Fig. 4 the staggered structure factor is graphed versus the temperature for various concentrations of ferromagnetic bonds. For $\rho = 2.5\%$ and 5%, $S(\pi, \pi)$ is significantly suppressed, but still has a temperature dependence similar to the clean system. For $\rho = 10\%$ the structure factor becomes almost temperature independent at $T \approx J/2$. This might be an indication that no long-range order exists for this concentration.

Figure 5 shows the enhancement of the uniform susceptibility as the disorder is increased. For comparison, $\rho = 0$ results for $L = 64$ are also shown. The finite-size effects for the uniform susceptibility are apparently quite small. The enhancement due to the presence of ferro-

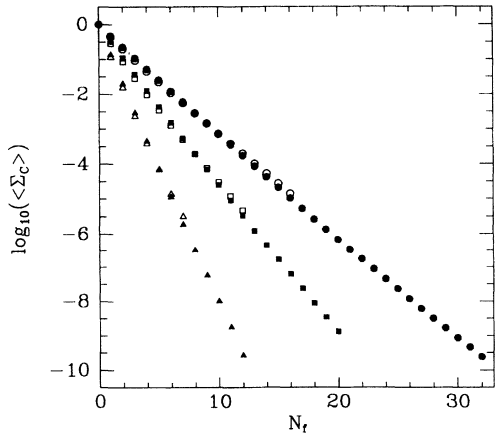

FIG. 3. The average sign vs the number of ferromagnetic bonds for $L = 4$ (open symbols) and $L = 8$ (solid symbols). Circles are for $T/J = 0.8$, squares for $T/J = 0.6$, and triangles for $T/J = 0.4$.

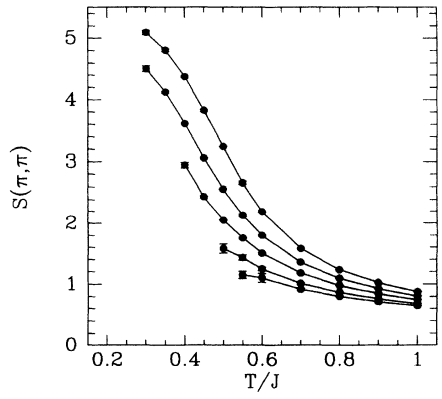

FIG. 4. The staggered structure factor for $L = 10$ vs the temperature for $\rho = 0\%$, 2.5%, 5%, 8%, and 10% (S decreasing with ρ).

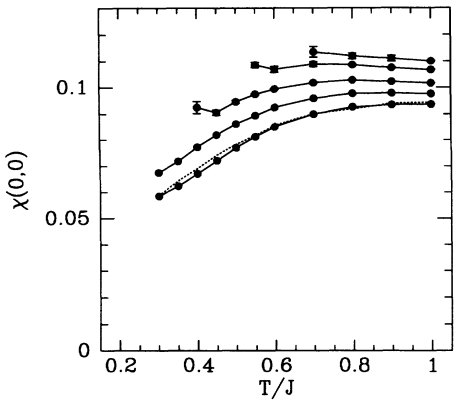

FIG. 5. The uniform susceptibility for $L = 10$ vs the temperature for $\rho = 0\%$, 2.5%, 5%, 8%, and 10% (χ increasing with ρ). The dashed curve goes through $\rho = 0$ results calculated for a system of size 64×64.

magnetic bonds is significant already for $\rho = 2.5\%$. As ρ is increased one would expect $\chi(0,0)$ to eventually diverge as $T \to 0$. There are indications of such behavior for $\rho \geq 5\%$, but unfortunately the sign problem limits the accuracy in this regime.

It is unclear whether low enough temperatures can be reached for determining the critical concentration using the scheme presented here. It should be possible, however, to carry out detailed studies for larger systems at temperatures above $T \approx J/4$ for concentrations of a few percent. This should enable an assessment of the relevance of the model to the high-T_c cuprates. The high-temperature regime is also important in view of the recent work on 2D quantum antiferromagnetism based on the nonlinear σ model.[11]

In summary, a scheme which alleviates the sign problem in quantum Monte Carlo simulations of the 2D quantum Heisenberg antiferromagnet with random ferromagnetic bonds has been presented. Results for the staggered structure factor and the uniform susceptibility show that the presence of a few percent of ferromagnetic bonds substantially suppresses the antiferromagnetism. The method discussed here can easily be extended for 3D systems.

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[1] S. Miyashita, M. Takasu, and M. Suzuki, in *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems*, edited by M. Suzuki (Springer-Verlag, Berlin, 1987).

[2] E.Y. Loh *et al.*, Phys. Rev. B **41**, 9301 (1990).

[3] A. Aharony *et al.*, Phys. Rev. Lett. **60**, 1330 (1988).

[4] J.E. Hirsch and R. Kariotis, Phys. Rev. B **32**, 7320 (1985); H.B. Schüttler, D.J. Scalapino, and P.M. Grant, *ibid.* **35**, 3461 (1987); S. Haas, J. Riera, and E. Dagotto, *ibid.* **48**, 13174 (1993).

[5] J. Behre and S. Miyashita, J. Phys. A **25**, 4745 (1992), E. Manousakis, Phys. Rev. B **45**, 7570 (1992); A.W. Sandvik and M. Vekić (unpublished).

[6] M. Guo, R.N. Bhatt, and D.A. Huse, Phys. Rev. Lett. **72**, 4137 (1994); H. Rieger and A.P. Young, *ibid.* **72**, 4141 (1994).

[7] S. Sachdev and J. Ye, Phys. Rev. Lett. **70**, 3339 (1993).

[8] A.W. Sandvik, J. Phys. A **25**, 3667 (1992).

[9] J. E. Hirsch *et al.*, Phys. Rev. B **26**, 5033 (1982).

[10] For large systems, care has to be taken in the evaluation of the average sign, as Σ_C can be very small relative to the individual terms of Eq. (16), and therefore highly sensitive to truncation errors.

[11] S. Chakravarty, B.I. Halperin, and D.R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988); S. Sachdev and J. Ye, *ibid.* **69**, 2411 (1992); A. Chubukov and S. Sachdev, *ibid.* **71**, 169 (1993).