

# Ground-state properties of the spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model on a square lattice by a Monte Carlo method

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The spin- $\frac{1}{2}$  antiferromagnetic Heisenberg model on a square lattice is studied by a Monte Carlo method. The ground-state energy and the lowest energies of the sectors  $S_z = 1$  and 2 are determined for lattice sizes ranging from  $4 \times 4$  to  $16 \times 16$ . The extrapolation to infinite lattice gives an energy per site equal to  $-0.6690 \pm 0.0002$ . The staggered magnetization was also measured for lattice sizes up to  $24 \times 24$ . The extrapolation to infinite lattice gives a value  $0.307 \pm 0.006$  in units where the saturated value is  $\frac{1}{2}$ .

## I. INTRODUCTION

The quantum antiferromagnetic Heisenberg model has raised much interest recently due to its connection to high- $T_c$  superconductivity.<sup>1,2</sup> In one dimension the spin- $\frac{1}{2}$  model does not possess long-range order. On a square lattice, however, numerical and analytical results indicate that the spin- $\frac{1}{2}$  model is ordered with a nonzero staggered magnetization which is about 60% of the classical value. Quantum fluctuations decrease the magnetization but do not destroy the long-range order.

On a square lattice the ground-state properties of the spin- $\frac{1}{2}$  model have been studied by several techniques such as spin-wave theory,<sup>3,4</sup> renormalization-group methods,<sup>5,6</sup> exact diagonalization,<sup>7-11</sup> and Monte Carlo methods.<sup>12-27</sup> Exact diagonalization has been carried out for small systems up to 32 sites.<sup>7-11</sup> Variational Monte Carlo methods,<sup>12-15</sup> finite-temperature path-integral Monte Carlo methods,<sup>16-20</sup> and zero-temperature Monte Carlo methods<sup>15,20-27</sup> were used to study larger systems.

In this paper we use a zero-temperature Monte Carlo method which has been applied previously to the antiferromagnetic Heisenberg chain.<sup>28</sup> The method differs from other zero-temperature Monte Carlo methods. These techniques are stochastic versions of the power method in which the largest eigenvalue of a matrix is obtained by repeated matrix multiplication. In the present method a probability distribution is defined which is proportional to a string of (non-negative) matrix elements such that the column index of an element equals the row index of the following element. The Metropolis algorithm is then used to estimate averages over the probability distribution so defined. If the string is long enough the averages will be dominated by the leading eigenvector of the matrix.

In the present method, the ground-state properties of a  $d$ -dimensional quantum spin system is seen as the statistical mechanical properties of a  $(d+1)$ -dimensional classical spin system. The extra dimension makes our method distinct from other zero-temperature Monte Carlo methods. Consider, for instance, the Green's-function Monte Carlo method.<sup>25,26</sup> It is based on the iteration of

the equation  $\psi_{n+1}(s') = \sum_s G(s', s) \psi_n(s)$ , where  $G$  is any function of the Hamiltonian that projects out the ground state. In order to use it as a stochastic process one has to decompose  $G(s', s)$  as the product of a transition probability  $P(s', s)$  and a multiplicity function  $m(s', s)$ . Our method avoids the need of the decomposition by the use of the extra dimension. Moreover, it is not necessary to make use of trial wave functions as is common in other zero-temperature Monte Carlo methods.

The numerical results we have obtained are in good agreement with results coming from exact diagonalization and other zero-temperature Monte Carlo methods. This is an indication that our method can give results that are at least as good as the ones obtained from other zero-temperature Monte Carlo methods. However, as happens to those methods, our scheme can be used only to treat those quantum problems for which the so-called "sign problem" is absent.

## II. THE METHOD

Consider a matrix  $T$  whose elements  $T(\tau_1, \tau_2)$  are non-negative and, for a fixed value of  $K$ , define a probability distribution  $P(\tau) = P(\tau_1, \tau_2, \dots, \tau_K)$  of the state  $\tau = (\tau_1, \tau_2, \dots, \tau_K)$ , apart from a normalization, by

$$P(\tau) \propto T(\tau_1, \tau_2) T(\tau_2, \tau_3) \cdots T(\tau_{K-1}, \tau_K) T(\tau_K, \tau_1). \quad (1)$$

The "interacting system" defined by this probability distribution is simulated by using the Metropolis algorithm. For  $K$  large enough the properties of the system are dominated by the leading eigenvector of  $T$ . The Monte Carlo simulation is possible to perform because the Metropolis algorithm requires only the ratio  $P(\tau')/P(\tau)$  of the probabilities of two states. From the Monte Carlo simulation one may obtain estimates of such averages as

$$\langle A(\tau_1) \rangle = \sum_{\tau_1} A(\tau_1) P(\tau_1) \quad (2)$$

and

$$\langle B(\tau_1, \tau_2) \rangle = \sum_{\tau_1} \sum_{\tau_2} B(\tau_1, \tau_2) P(\tau_1, \tau_2), \quad (3)$$

where  $P(\tau_1)$  and  $P(\tau_1, \tau_2)$  are marginal probability distributions obtained from  $P(\tau)$ , defined by

$$P(\tau'_1) = \sum_{\tau} \delta(\tau'_1, \tau_1) P(\tau) \quad (4)$$

and

$$P(\tau'_1, \tau'_2) = \sum_{\tau} \delta(\tau'_1, \tau_1) \delta(\tau'_2, \tau_2) P(\tau). \quad (5)$$

The matrix  $T$  is considered to be irreducible (that is, the elements of  $T^k$  are strictly positive for  $k$  larger than a certain value) so that the Perron-Frobenius theorem guaranties that its largest eigenvalue  $\lambda_0$  will be nondegenerate and the corresponding eigenvector  $\phi_0$  will have positive elements, that is,  $\phi_0(\tau_1) > 0$ . When  $K$  is large the marginal probability distributions  $P(\tau_1)$  and  $P(\tau_1, \tau_2)$  will be related to the leading eigenvector  $\phi_0$  by

$$P(\tau_1) = [\phi_0(\tau_1)]^2 \quad (6)$$

and

$$P(\tau_1, \tau_2) = \lambda_0^{-1} \phi_0(\tau_1) T(\tau_1, \tau_2) \phi_0(\tau_2), \quad (7)$$

the corrections being of the order  $(\lambda_1/\lambda_0)^K$  where  $\lambda_1$  is the second largest eigenvalue of  $T$ .

From Eqs. (4) and (5) we get the equation

$$P(\tau_1, \tau_1) = \lambda_0^{-1} T(\tau_1, \tau_1) P(\tau_1) \quad (8)$$

which can be used to obtain the following formula:

$$\lambda_0 = \frac{\langle T(\tau_1, \tau_1) \rangle}{\langle \delta(\tau_1, \tau_2) \rangle}. \quad (9)$$

This formula permits the calculation of the largest eigenvalue of  $T$  from the estimates of  $\langle T(\tau_1, \tau_1) \rangle$  and  $\langle \delta(\tau_1, \tau_2) \rangle$  obtained from the Monte Carlo simulation.

### III. THE MATRIX $T$

The method is applied to the spin- $\frac{1}{2}$  antiferromagnetic Heisenberg Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (10)$$

where the sum is over the nearest-neighbor pairs of sites on a square lattice of  $N$  sites. To get a non-negative matrix we perform a canonical transformation on  $\mathcal{H}$  by letting  $S_i^x \rightarrow -S_i^x$ ,  $S_i^y \rightarrow -S_i^y$ , and  $S_i^z \rightarrow S_i^z$  if site  $i$  belongs to one of the sublattices and leaving the spins of the other sublattice invariant. The transformed Hamiltonian will be then

$$\mathcal{H} = - \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y - S_i^z S_j^z). \quad (11)$$

Now, if we consider the operator  $\mathcal{T} = -2\mathcal{H} + N_p/2$ , where  $N_p$  is the number of nearest-neighbor pairs of sites on the lattice, the eigenvalues  $E$  of  $\mathcal{H}$  and  $\lambda$  of  $\mathcal{T}$  are related by  $E = -\lambda/2 + N_p/4$ , so that the largest eigenvalue of  $\mathcal{T}$  will be related to the ground-state energy of  $\mathcal{H}$ . The operator  $\mathcal{T}$  is given by

$$\mathcal{T} = 2 \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) + 2 \sum_{\langle ij \rangle} (\frac{1}{4} - S_i^z S_j^z). \quad (12)$$

In the  $S^z$  representation, the elements  $T(\sigma, \sigma') = \langle \sigma | \mathcal{T} | \sigma' \rangle$ ,  $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_N)$ ,  $\sigma_i = \pm 1$ , are non-negative. The matrix  $T$  is block diagonal and each block is characterized by the eigenvalue  $M$  of  $S^z = S_1^z + S_2^z + \dots + S_N^z$ . Moreover, each block is irreducible so that the present Monte Carlo method can be used to calculate the largest eigenvalue within each block. A nondiagonal element is either zero or one. It equals one when  $\sigma'$  and  $\sigma$  differ by just one pair of nearest-neighbor sites having antiparallel spins, and vanishes otherwise. A diagonal element  $T(\sigma, \sigma)$  equals the number of pairs of nearest-neighbor sites with antiparallel spins in the configuration  $\sigma$ .

### IV. MONTE CARLO ALGORITHM

The Monte Carlo algorithm is defined as follows. We consider a cubic lattice of  $N \times K$  sites composed of  $K$  layers each layer being a square lattice of  $L \times L = N$  sites. At each site there is a spin variable  $\sigma_{ik} = \pm 1$ , where the index  $k = 1, 2, \dots, K$  indicates the layer and the index  $i$  the position of the site within the layer. One starts with a configuration  $\{\sigma_{ij}\}$  such that (a) for each layer  $k$  one has  $\sum_i \sigma_{ik} = 2M$ , and such that (b) two consecutive layers differ at most by one pair of nearest-neighbor antiparallel spins. This must be so otherwise the product on Eq. (1) would vanish. The Monte Carlo algorithm is constructed in such a way that these two properties are preserved in each step of the simulation.

At each time step of the Monte Carlo simulation we first choose a layer at random, say layer  $k$ , and try to modify its configuration according to the following cases.

(1) The chosen layer is identical to the preceding and following layers. Then we pick up at random one of the  $A_k$  pairs of nearest-neighbor antiparallel spins of the chosen layer. The two spins of the pair are then exchanged with probability  $1/A_k$ .

(2) The preceding layer ( $k-1$ ) is identical to the following layer ( $k+1$ ) but distinct from the chosen layer ( $k$ ) which differs from the other two by just one pair of nearest-neighbor antiparallel spins. In this case the two spins of the pair are just exchanged and the chosen layer becomes identical to the other two layers.

(3) The preceding layer ( $k-1$ ) is identical to the chosen layer ( $k$ ) but distinct from the following layer ( $k+1$ ). The chosen layer differs from the following layer by just one pair of nearest-neighbor antiparallel spins. In this case the two spins of the pair are exchanged with probability  $\min\{1, A_{k+1}/A_{k-1}\}$ .

(4) The following layer ( $k+1$ ) is identical to the chosen layer ( $k$ ) but distinct from the preceding layer ( $k-1$ ). The chosen layer differs from the preceding layer by just one pair of nearest-neighbor antiparallel spins. In this case the two spins of the pair are exchanged with probability  $\min\{1, A_{k-1}/A_{k+1}\}$ .

(5) The three layers ( $k-1$ ,  $k$ , and  $k+1$ ) are distinct from each other. The chosen layer differs from the preceding and following layer by two distinct pairs of

nearest-neighbor antiparallel spins. In this case we consider the following subcases.

(5a) The two spins do not belong to the same plaquette of four spins. In this case the spins within each pair are exchanged if the pairs do not have one site in common.

(5b) The two pairs belong to the same plaquette and have one site in common, that is, the bonds that connect the spins are perpendicular. If the sum of the four spins belonging to the plaquette is zero, then these four spins are flipped. Otherwise, we flip only the spin of the common site and the spin of the diagonally opposite site.

(5c) The two pairs belong to the same plaquette and do not have any site in common, that is, the bonds that connect the spins within each pair are parallel. If the two spins belonging to the one of the diagonals of the plaquette have the same sign, the four spins are flipped. Otherwise, we choose randomly one of the diagonals of the plaquette and flip the two spins belonging to the chosen diagonal.

It is straightforward, although tedious, to verify that the transition probabilities defined by the above algorithm satisfy detailed balance for a stationary probability given by Eq. (2).

## V. RESULTS

Using the algorithm of the previous section we have calculated the largest eigenvalue within each one of the blocks  $M=0, 1$ , and  $2$ , for  $L=4, 6, 8, 12$ , and  $16$  by using Eq. (9). The staggered magnetization was also estimated for these values and for  $L=10$  and  $24$ . We used lattices with  $K$  ranging from 2000 to 4000. We have checked our method for the case  $L=4$  by comparing our result with existing results obtained by exact diagonalization [8].

The ground-state energy per site  $E_0/L^2$ , the first excited state energy per site  $E_1/L^2$ , and the spin-2 state energy per site  $E_2/L^2$  are displayed in Table I for lattice sizes ranging from  $L=4$  to  $16$ . The energy per site  $E_0/L^2$ ,  $E_1/L^2$ , and  $E_2/L^2$  are plotted in Fig. 1 as a function of  $(1/L)^3$ . Assuming the behavior  $E_M/L^2 = \epsilon + c_M/L^3$ ,  $M=0, 1, 2$ , the linear fitting to the data points gives  $\epsilon = -0.6690 \pm 0.0002$ ,  $c_0 = -2.07 \pm 0.02$ ,  $c_1 = 0.22 \pm 0.02$ , and  $c_2 = 3.18 \pm 0.07$ . The extrapolated value for the energy per site  $-0.6690 \pm 0.0002$  and the slope constant  $2.07 \pm 0.02$  are in good agreement with results obtained by Carlson [25],  $-0.66918(10)$  and  $2.086$ ; Trivedi and

TABLE I. Ground-state energy per site  $E_0/L^2$ , first excited state energy per site  $E_1/L^2$ , and lowest-energy per site  $E_2/L^2$  for states with  $M=2$  calculated by the present Monte Carlo method.

$L$	$E_0/L^2$	$E_1/L^2$	$E_2/L^2$
4	-0.7018(3)	-0.6652(3)	-0.5943(2)
6	-0.6783(2)	-0.6704(4)	-0.6539(3)
8	-0.6715(3)	-0.6703(6)	-0.6647(4)
12	-0.6699(3)	-0.6692(4)	-0.6680(8)
16	-0.6700(6)	-0.6681(10)	-0.6677(12)
$\infty$	-0.6690(2)	-0.6690(2)	-0.6690(2)

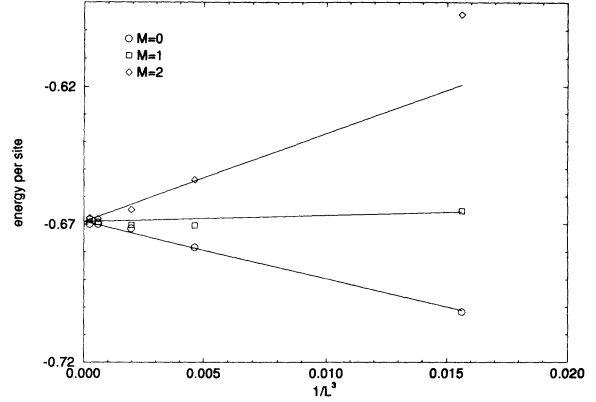


FIG. 1. Ground-state energy per site  $E_0/L^2$ , and lowest energies per site  $E_1/L^2$  and  $E_2/L^2$  of the sectors  $M=1$  and  $2$ , respectively, as a function of  $1/L^3$ . The straight lines are linear fittings to the Monte Carlo data points.

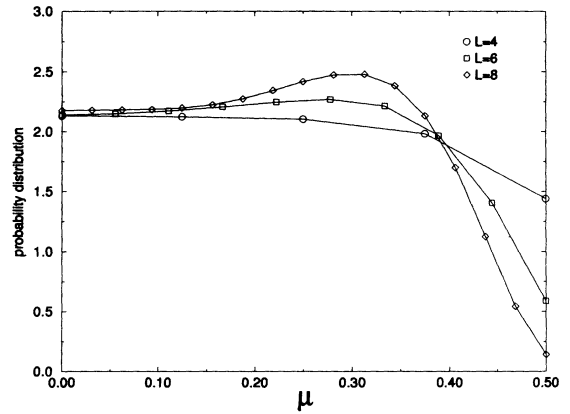


FIG. 2. Probability distribution of the  $z$  component of the staggered magnetization  $\mu$  for  $L=4, 6, 8$ .

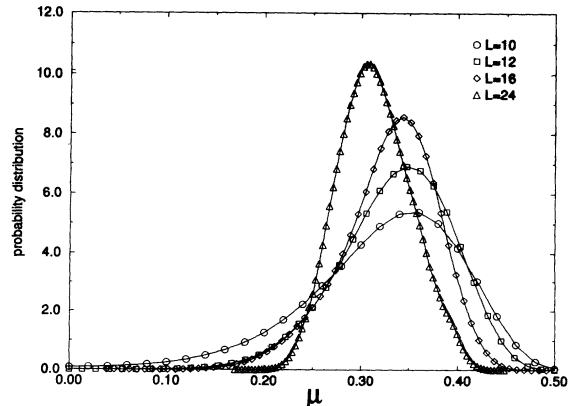


FIG. 3. Probability distribution of the  $z$  component of the staggered magnetization  $\mu$  for  $L=10, 12, 16, 24$ .

TABLE II. This table shows the  $z$  component of the staggered magnetization  $m_z^*$  and  $m_z^\dagger$  for several values of  $L$  for the ground state.

$L$	$m_z^*$	$m_z^\dagger$
4	0.2587(6)	0.3036(5)
6	0.234(3)	0.274(3)
8	0.261(8)	0.288(6)
10	0.323(4)	0.333(3)
12	0.322(4)	0.328(3)
16	0.318(4)	0.323(4)
24	0.314(6)	0.317(6)
$\infty$	0.307(6)	0.307(6)

Capeley [26],  $-0.6692(2)$  and  $2.08(2)$ ; and Barnes and Kovarick [27],  $-0.66923(13)$  and  $2.083(8)$ . These results were obtained by using zero-temperature Monte Carlo Methods distinct from ours.

The appropriate order parameter for the present system is the ground-state staggered magnetization per site defined by

$$\mathbf{m} = \left\langle \psi_0 \left| \frac{1}{L^2} \sum_i \epsilon_i \mathbf{S}_i \right| \psi_0 \right\rangle, \quad (13)$$

where  $\epsilon_i$  is 1 if site  $i$  belongs to one of the sublattices and  $-1$  if it belongs to the other. However, one expects  $\mathbf{m}$  to vanish since finite lattices cannot have spontaneous symmetry breaking. Therefore, one considers, instead, the root-mean-square staggered magnetization  $m^\dagger$  defined by

$$m^\dagger = \left[ \left\langle \psi_0 \left| \left[ \frac{1}{L^2} \sum_i \epsilon_i \mathbf{S}_i \right]^2 \right| \psi_0 \right\rangle \right]^{1/2}. \quad (14)$$

In actual calculation we have measured its  $z$  projection  $m_z^\dagger$  given by

$$m_z^\dagger = \left[ \left\langle \psi_0 \left| \left[ \frac{1}{L^2} \sum_i \epsilon_i S_i^z \right]^2 \right| \psi_0 \right\rangle \right]^{1/2}. \quad (15)$$

In the isotropic ground state of the finite lattices the three components are the same so that  $m^\dagger = \sqrt{3}m_z^\dagger$ . That is exactly what actually happens in the simulation for the cases  $L=4, 6, 8$ . However, for larger values of  $L$ , the Monte Carlo results, obtained by starting with a configuration with a saturated staggered magnetization in the  $z$  direction, show that the isotropy is broken and that the system exhibits a staggered magnetization in the  $z$  direction. This is shown in Figs. 2 and 3 where the probability distribution  $P_L(\mu)$  of the variable  $\mu = L^{-2} \sum_i \epsilon_i \frac{1}{2} \sigma_i$  is displayed for  $L=4, 6, 8, 10, 12, 16$ , and 24.

Table II shows  $m_z^* = \sum |\mu| P_L(\mu)$  and  $m_z^\dagger = [\sum \mu^2 P_L(\mu)]^{1/2}$  for several values of  $L$ . For  $L=10, 12,$

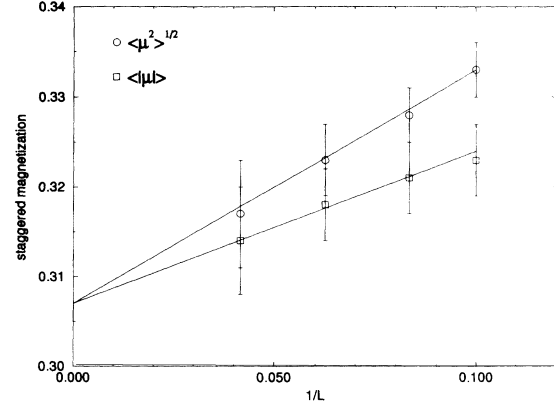


FIG. 4. Staggered magnetization as a function of  $1/L$ . The straight lines are linear fittings to the Monte Carlo data points.

16, and 24, the staggered magnetization is identified with the staggered magnetization in the  $z$  direction  $m_z^\dagger$ . For  $L=4, 6, 8$  the results are to be multiplied by  $\sqrt{3}$ . Figure 4 shows  $m_z^\dagger$  and  $m_z^*$  as a function of  $1/L$ . Assuming the behavior  $m_z^\dagger = m + a/L$  and  $m_z^* = m + b/L$ , the extrapolation to infinite lattice gives  $m = 0.307(6)$ .

## VI. CONCLUSION

We have studied the spin- $\frac{1}{2}$  antiferromagnetic Heisenberg model on a square lattice by a zero-temperature Monte Carlo Method. We have calculated the ground-state energy as well as the lowest energies of the sectors  $S_z=1$  and 2 for lattice sizes ranging from  $4 \times 4$  to  $16 \times 16$ . The staggered magnetization was also measured for lattice sizes up to  $24 \times 24$ . The value of the extrapolated energy per site  $-0.6690 \pm 0.0002$  and the staggered magnetization  $0.307 \pm 0.006$  are in good agreement with results obtained by other zero-temperature Monte Carlo methods.

In the present method, the ground-state properties of the two-dimensional quantum antiferromagnetic Heisenberg model is represented by a three-dimensional classical spin system. The extra dimension makes our method distinct from other zero-temperature Monte Carlo methods by avoiding the need to decompose the projector into a transition probability and a multiplicity function. The numerical results indicate that the method can give results that are at least as good as the ones obtained from other zero-temperature Monte Carlo methods.

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<sup>1</sup>E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

<sup>2</sup>T. Barnes, Int. J. Mod. Phys. C **2**, 659 (1991).

<sup>3</sup>R. Kubo, Phys. Rev. **87**, 568 (1952).

<sup>4</sup>H. Nishimori and S. J. Miyake, Prog. Theor. Phys. **73**, 18

(1985).

<sup>5</sup>C. Y. Pan, Int. J. Mod. Phys. B **3**, 1435 (1989).

<sup>6</sup>H. Q. Lin and D. Campbell, Phys. Rev. Lett. **69**, 2415 (1992).

<sup>7</sup>J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978).

- <sup>8</sup>S. Tang and J. E. Hirsch, *Phys. Rev. B* **39**, 4548 (1989).  
<sup>9</sup>E. Dagotto and A. Moreo, *Phys. Rev. B* **39**, 4744 (1989).  
<sup>10</sup>M. Kikuchi and Y. Okabe, *J. Phys. Soc. Jpn.* **58**, 679 (1989).  
<sup>11</sup>H. Q. Lin, *Phys. Rev. B* **42**, 6561 (1990).  
<sup>12</sup>D. A. Huse and V. Elser, *Phys. Rev. Lett.* **60**, 2531 (1988).  
<sup>13</sup>H. Yokoyama and H. Shiba, *J. Phys. Soc. Jpn.* **56**, 3570 (1987).  
<sup>14</sup>S. Liang, B. Douçout, and P. W. Anderson, *Phys. Rev. Lett.* **61**, 365 (1988).  
<sup>15</sup>S. Liang, *Phys. Rev. B* **42**, 6555 (1990).  
<sup>16</sup>J. D. Reger and A. P. Young, *Phys. Rev. B* **37**, 5978 (1988).  
<sup>17</sup>Y. Okabe and M. Kikuchi, *J. Phys. Soc. Jpn.* **57**, 4351 (1988).  
<sup>18</sup>Y. Okabe and M. Kikuchi, *J. Phys. C* **8**, 1393 (1988).  
<sup>19</sup>J. D. Reger, J. A. Riera, and A. P. Young, *J. Phys. Condens. Matter* **1**, 1855 (1989).  
<sup>20</sup>M. Gross, E. Sanchez-Velasco, and E. Siggia, *Phys. Rev. B* **39**, 2484 (1989).  
<sup>21</sup>M. Gross, E. Sanchez-Velasco, and E. Siggia, *Phys. Rev. B* **40**, 11 328 (1989).  
<sup>22</sup>N. Trivedi and D. M. Ceperley, *Phys. Rev. B* **40**, 2737 (1989).  
<sup>23</sup>T. Barnes and E. S. Swanson, *Phys. Rev. B* **37**, 9405 (1988).  
<sup>24</sup>T. Barnes, D. Kotchan, and E. S. Swanson, *Phys. Rev. B* **39**, 9357 (1989).  
<sup>25</sup>J. Carlson, *Phys. Rev. B* **40**, 846 (1989).  
<sup>26</sup>N. Trivedi and D. M. Ceperley, *Phys. Rev. B* **41**, 4552 (1990).  
<sup>27</sup>T. Barnes and M. D. Kovařik, *Phys. Rev. B* **42**, 6159 (1990).  
<sup>28</sup>M. J. de Oliveira, *Phys. Rev. B* **48**, 6141 (1993).