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Forward-walking Green's Function Monte Carlo Method for Correlation Functions

M. Samaras and C. J. Hamer

School of Physics, University of New South Wales,
Sydney, NSW 2052, Australia.
mrrs@newt.phys.unsw.edu.au, cjh@newt.phys.unsw.edu.au

Abstract

The forward-walking Green's Function Monte Carlo method is used to compute expectation values for the transverse Ising model in $(1+1)D$, and the results are compared with exact values. The magnetisation M_z and the correlation function $\rho^z(n)$ are computed. The algorithm reproduces the exact results, and convergence for the correlation functions seems almost as rapid as for local observables such as the magnetisation. The results are found to be sensitive to the trial wavefunction, however, especially at the critical point.

1. Introduction

Monte Carlo methods are a powerful and effective tool for exploring the behaviour of complicated systems, and their use is increasing rapidly in every area of physics. Here we are interested in quantum Hamiltonian lattice systems, particularly quantum spin models and 'Hamiltonian' lattice gauge theories (Kogut and Susskind 1975). The use of quantum Monte Carlo methods (Ceperley and Kalos 1979; Ceperley 1997) has not been very extensive in these areas as yet; although some lengthy and accurate studies of the Heisenberg antiferromagnet on the square lattice have appeared recently (Trivedi and Ceperley 1990; Runge 1992*a*, 1992*b*; Sandvik 1997; Sorella 1998). In particular there have been very few attempts to calculate correlation functions in these models by Monte Carlo techniques. Yet the calculation of correlation functions is essential: for instance, it is the only way to reliably extract information about the bound-state spectrum in lattice gauge theories within a weak-coupling representation, for both the Euclidean and Hamiltonian formulations (Hamer *et al.* 1996).

Trivedi and Ceperley (1990) did calculate ground-state correlations in the case of the $S = \frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. They used a 'mixed' estimator for the correlation function, which involves taking the overlap of the stochastic Monte Carlo 'wave function' with a trial state $|\Psi_T\rangle$. The method appears to work very well in this case, by comparison with other approaches. Nevertheless, it is intrinsically a 'biased' estimate, depending on the quality of the trial wavefunction $|\Psi_T\rangle$. They find that it is essential to include the zero-point motion of the elementary excitations (spin waves) in this case in order to obtain long-range correlations in the trial wavefunction.

Our aim in this paper is to try out a different Monte Carlo method for the calculation of correlation functions, by testing it on a case where some exact analytic results are already known, namely the transverse Ising model in $(1+1)$ dimensions. This is the quantum Hamiltonian corresponding to the classical $2D$ Ising model and has been used as a test-bed for many numerical techniques. The method we shall use is the ‘forward-walking’ method (Liu *et al.* 1974; Whitlock *et al.* 1979; Kalos 1966) in conjunction with the so-called Green’s Function Monte Carlo algorithm (Ceperley and Kalos 1979), as used by Trivedi and Ceperley (1990) or Runge (1992*a*, 1992*b*) to calculate the ground-state energy and magnetisation for the Heisenberg antiferromagnet on a square lattice. The forward-walking method does not depend explicitly on any trial state $|\Psi_T\rangle$, as the mixed-estimate method does; although one generally uses a trial state to ‘guide’ the Monte Carlo random walk towards the most important regions of configuration space (Ceperley and Kalos 1979), as we shall see later.

There are no new physical results in the paper, but we believe it is a useful exercise to show that the GFMC method combined with forward-walking techniques can give correct results for the correlation functions, as compared with the known exact results in this model. There is also a discussion of the asymptotic behaviour of the correlation functions which should be of some pedagogical value. In Section 2 the exactly known analytic results relevant to these calculations are summarised. The Monte Carlo algorithms are outlined in Section 3, and results are presented in Section 4. Finally, our conclusions are given in Section 5.

2. Analytic Results

The $(1+1)D$ or ‘transverse’ Ising model has the quantum Hamiltonian

$$H = \sum_{m=1}^M [1 - \sigma_z(m)] - x \sum_{m=1}^M \sigma_x(m) \sigma_x(m+1), \quad (1)$$

where the index m labels sites on a one-dimensional chain of M sites, while the $\sigma_i(m)$ are Pauli matrices acting on a two-state spin variable at each site. Periodic boundary conditions will be assumed throughout.

In the bulk limit $M \rightarrow \infty$, this Hamiltonian has been solved by Pfeuty (1970), using the methods of Lieb *et al.* (1961, 1964). The spin Hamiltonian is transformed to a fermionic Hamiltonian by means of a Jordan–Wigner transformation, and the resulting quadratic form in fermion operators is diagonalised by a Bogoliubov transformation.

Finite-size corrections have been discussed by a number of authors (Nightingale 1976; Cardy 1988): for a review see Christe and Henkel (1993). The ground state energy of the system is given by

$$E_0 = M - \sum_{k=0}^{M-1} \Lambda(\theta_k^+), \quad (2)$$

where

$$\Lambda(\theta) = [1 + x^2 + 2x \cos \theta]^{\frac{1}{2}}, \quad (3)$$

$$\theta_k^+ = \begin{cases} \frac{(2k+1)\pi}{M} & (M \text{ even}) \\ \frac{2k\pi}{M} & (M \text{ odd}) \end{cases} \quad (4)$$

while the energy of the first excited state is

$$E_1 = 2(1-x) + M - \sum_{k=0}^{M-1} \Lambda(\theta_k^-), \quad (5)$$

with

$$\theta_k^- = \begin{cases} \frac{(2k+1)\pi}{M} & (M \text{ odd}) \\ \frac{2k\pi}{M} & (M \text{ even}) \end{cases} \quad (6)$$

In the bulk limit, the ground-state energy per site is given in terms of an elliptic integral:

$$\epsilon_0 = \lim_{M \rightarrow \infty} \left(\frac{E_0}{M} \right) = 1 - \frac{2(1+x)}{\pi} E \left(\frac{4x}{(1+x)^2} \right), \quad (7)$$

and the energy gap is exactly

$$E_1 - E_0 = 2(1-x) \quad (x < 1), \quad (8)$$

This gap vanishes at the critical coupling $x = 1$.

Spacelike Correlation Functions

Expressions for the spacelike correlation functions have also been obtained by Pfeuty (1970). Let

$$M_z = \langle 0 | \sigma_z(m) | 0 \rangle \quad (9)$$

and

$$\rho^x(n) = \langle 0 | \sigma_x(m) \sigma_x(m+n) | 0 \rangle \quad (10)$$

$$\rho^y(n) = \langle 0 | \sigma_y(m) \sigma_y(m+n) | 0 \rangle \quad (11)$$

$$\rho^z(n) = \langle 0 | \sigma_z(m) \sigma_z(m+n) | 0 \rangle \quad (12)$$

(these definitions differ from Pfeuty's by a factor of 2). Then Pfeuty's results are

$$M_z = G(0), \quad (13)$$

$$\rho^z(n) = M_z^2 - G(n)G(-n), \quad (14)$$

$$\rho^x(n) = \begin{vmatrix} G(-1) & G(-2) & \dots & G(-n) \\ G(0) & G(-1) & \dots & G(-n+1) \\ \dots & & & \\ G(n-2) & & \dots & G(-1) \end{vmatrix}, \quad (15)$$

$$\rho^y(n) = \begin{vmatrix} G(1) & G(0) & \dots & G(2-n) \\ G(2) & & \dots & G(3-n) \\ \dots & & & \\ G(n) & & \dots & G(1) \end{vmatrix}, \quad (16)$$

with

$$G(n) = L(n) + xL(n+1), \quad (17)$$

$$L(n) = \frac{1}{M} \sum_{k=0}^{M-1} \frac{\cos(n\theta_k^+)}{\Lambda(\theta_k^+)}, \quad (18)$$

or in the bulk limit where $M \rightarrow \infty$

$$L(n) = \frac{1}{\pi} \int_0^\pi dk \frac{\cos(kn)}{\Lambda(k)}. \quad (19)$$

We shall be particularly interested in the ‘connected’ correlation function

$$\rho_c^z(n) = \rho^z(n) - M_z^2. \quad (20)$$

The asymptotic behaviour of these functions can be found by adapting the results of Barouch and McCoy (1971), which were obtained for a more general spin- $\frac{1}{2}$ XY model in a magnetic field. We consider various cases.

The critical point $x = 1$

At the critical point, a number of results can be obtained in closed form. The ground-state energy per site is (Hamer and Barber 1981)

$$\epsilon_0 = \frac{E_0}{M} = 1 - \frac{2}{M} \csc\left(\frac{\pi}{2M}\right) \quad (21)$$

$$\underset{M \rightarrow \infty}{\sim} 1 - \frac{4}{\pi} - \frac{\pi}{6M^2} + O(M^{-4}), \quad (22)$$

while the energy gap is (Hamer and Barber 1981)

$$\Delta E = E_1 - E_0 = 2 \tan \left(\frac{\pi}{4M} \right) \quad (23)$$

$$\underset{M \rightarrow \infty}{\sim} \frac{\pi}{2M} + O(M^{-3}). \quad (24)$$

The leading-order finite-size corrections have been exhibited in these formulae, which may be compared with the predictions of conformal invariance theory (Christe and Henkel 1993):

$$\epsilon_0(M) - \epsilon_0(\infty) \underset{M \rightarrow \infty}{\sim} -\frac{\pi c v}{6M^2} \quad (25)$$

and

$$\Delta E \underset{M \rightarrow \infty}{\sim} \frac{2\pi x v}{M}, \quad (26)$$

where c is the central charge, v is the ‘speed of light’, and x is the relevant scaling index. For the transverse Ising model $c = \frac{1}{2}$ and $x = \frac{1}{8}$ for the magnetic scaling index, which shows that the speed of light $v = 2$ for this particular Hamiltonian.

The function $G(n)$ reduces to

$$G(n) = \frac{(-1)^n}{M \sin[(n + \frac{1}{2})\pi/M]} \quad (27)$$

and hence

$$M_z = \frac{1}{M \sin(\pi/2M)} \underset{M \rightarrow \infty}{\sim} \frac{2}{\pi}, \quad (28)$$

and

$$\rho_c^z(n) = \frac{2}{M^2 [\cos(\pi/M) - \cos(2n\pi/M)]}. \quad (29)$$

In the bulk limit $M \rightarrow \infty$ with n finite, the correlation functions reduce to (Pfeuty 1970)

$$\rho_c^z(n) \underset{M \rightarrow \infty}{\sim} \frac{4}{\pi^2 (4n^2 - 1)}, \quad (30)$$

$$\rho^x(n) \underset{M \rightarrow \infty}{\sim} \left(\frac{2}{\pi} \right)^n 2^{2n(n-1)} \frac{H(n)^4}{H(2n)} \quad (31)$$

with

$$H(n) = 1^{n-1} 2^{n-2} \dots (n-1), \quad (32)$$

whence (Wu 1966)

$$\rho^x(n) \stackrel{M \rightarrow \infty}{\sim} n^{-1/4} e^{1/4} 2^{1/12} A^{-3}, \quad (33)$$

where $A = 1.282\dots$ is Glaisher's constant: and

$$\rho^y(n) \stackrel{M \rightarrow \infty}{\sim} -\frac{\rho^x(n)}{4n^2 - 1}. \quad (34)$$

In the 'continuum' limit $M \rightarrow \infty$, $\tau = n/M$ finite, we find

$$\rho_c^z(n) \stackrel{M \rightarrow \infty}{\sim} \frac{1}{[M \sin(\pi\tau)]^2}, \quad (35)$$

which is precisely the form predicted by the theory of conformal invariance (Cardy 1984, 1990).

Régime $x < 1$

This is the 'high-temperature' régime in which there is no ferromagnetic order in the x -direction. In the bulk limit $M \rightarrow \infty$, n finite, the function $G(n)$ becomes

$$G(n) \stackrel{M \rightarrow \infty}{\rightarrow} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq e^{iqn} \left[\frac{1 + x e^{iq}}{1 + x e^{-iq}} \right]^{\frac{1}{2}}. \quad (36)$$

Writing this as a contour integral, contracting the contour onto the cut from $z + e^{iq} = 0$ to $z = -x$, and expanding about $z = -x$, one finds for large n

$$G(n) \rightarrow \frac{(-1)^n}{\pi} x^n \left[(1 - x^2)^{\frac{1}{2}} B(n + \tfrac{1}{2}, \tfrac{1}{2}) + \frac{x^2}{2(1 - x^2)^{\frac{1}{2}}} B(n + \tfrac{1}{2}, \tfrac{3}{2}) + \dots \right] \quad (37)$$

and similarly

$$G(-n) \sim \frac{(-1)^{n-1}}{\pi} x^n \left[\frac{1}{(1 - x^2)^{\frac{1}{2}}} B(n - \tfrac{1}{2}, \tfrac{3}{2}) - \frac{x^2}{2(1 - x^2)^{\frac{3}{2}}} B(n - \tfrac{1}{2}, \tfrac{5}{2}) + \dots \right] \quad (38)$$

and hence

$$\rho_c^z(n) \stackrel{n \rightarrow \infty}{\sim} \frac{x^{2n}}{2\pi n^2} [1 + O(n^{-1})] \quad (39)$$

as previously derived by Barouch and McCoy (1971) (up to an overall sign). They also find

$$\rho^x(n) \underset{n \rightarrow \infty}{\sim} \frac{x^n}{\sqrt{\pi n}} (1-x^2)^{-\frac{1}{4}} [1 + O(n^{-1})], \quad (40)$$

$$\rho^y(n) \sim -\frac{x^n}{2\sqrt{\pi n^3}} (1-x^2)^{\frac{3}{4}} [1 + O(n^{-1})]. \quad (41)$$

We want to compare these results with the exponentially decreasing behaviour

$$\rho(n) \sim \exp \left[-n \frac{\Delta E}{v} \right] \quad (42)$$

expected for a general correlation function, where ΔE is the energy gap, and v is the ‘speed of light’, or anisotropy parameter between space and time. Near $x = 1$, the result of equation (39) can be rewritten as

$$\rho_c^z(n) \underset{n \rightarrow \infty}{\sim} \frac{1}{2\pi n^2} e^{2n \ln(x)} \quad (43)$$

$$\underset{x \rightarrow 1}{\sim} \frac{1}{2\pi n^2} e^{-2n(1-x)}. \quad (44)$$

For the operator σ_z , the relevant energy gap is that in the vacuum sector, i.e. $\Delta E = 4(1-x)$, and so equation (43) corresponds to equation (42) provided that the speed of light $v = 2$, as already deduced from the finite size corrections (or alternatively from the dispersion relation of the excitations at $x = 1$). For the correlation function $\rho^x(n)$ the exponent is only half as big, because there the relevant gap is the even-odd gap, $\Delta E = 2(1-x)$. Thus the ansatz equation (42) holds good in the neighbourhood of the ‘continuum limit’, i.e. the critical point $x = 1$. Away from that region, however, the ansatz breaks down: one can no longer treat the model as an anisotropic continuum system.

Where the ansatz (42) holds, we may hope to estimate the energy gap from measurements of the spacelike correlation functions, provided that the speed of light is known. The presence of the power-law terms such as the factor $1/n^2$ in equation (43) tends to complicate the process, however, and makes it more difficult to obtain a phenomenological exponent value from measurements of the correlation functions. This may be illustrated as follows. Assuming the correlation function $\rho(n) \sim \exp(-n/\xi)$, a naive estimate of the correlation length is

$$R(n) = \ln \left[\frac{\rho(n)}{\rho(n+1)} \right] \underset{n \rightarrow \infty}{\sim} \frac{1}{\xi}. \quad (45)$$

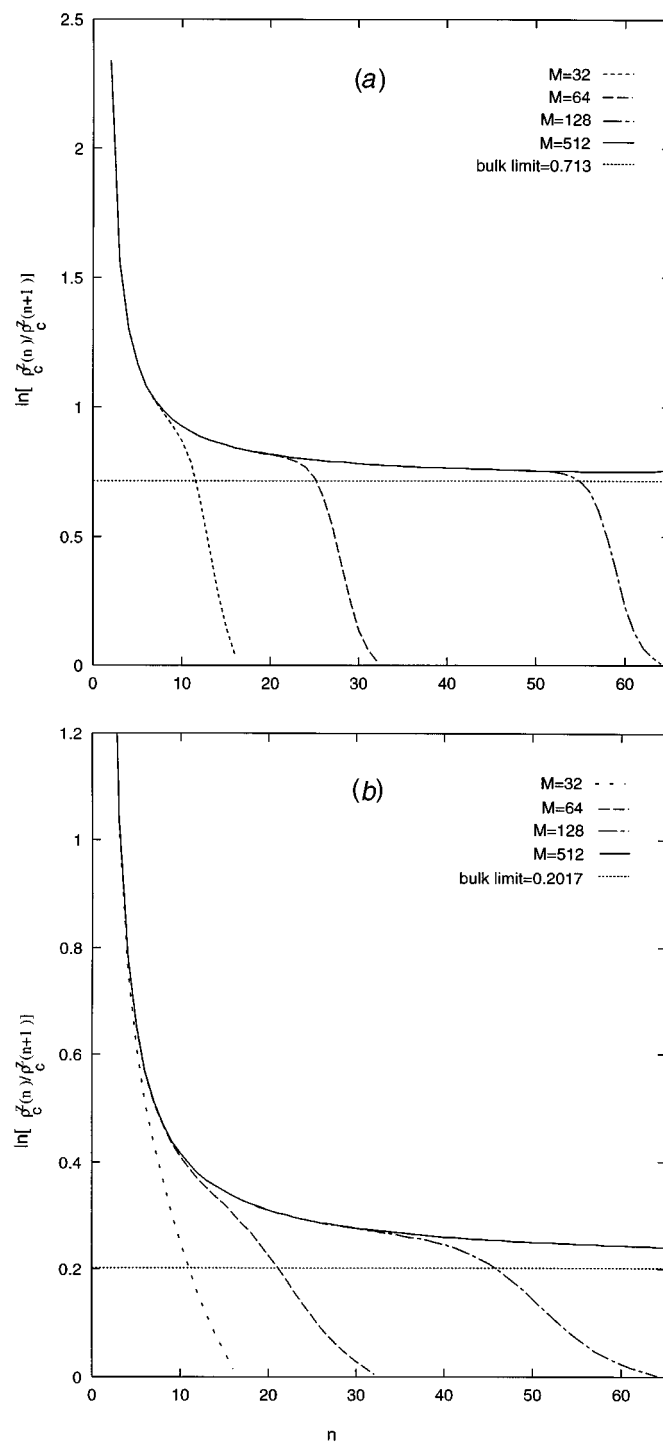


Fig. 1. The ratio $R(n)$ plotted against n for lattice sizes 32, 64 and 128 at: (a) $x = 0.7$ and (b) $x = 0.9$. The asymptotic value is shown as a horizontal line.

Fig. 1 shows the value of the quantity $R(n)$ as a function of n , calculated for the correlation function $\rho_c^z(n)$, at (a) $x = 0.7$ and (b) $x = 0.9$. The exact results (from equation 12) for lattice sizes 32, 64 and 128 are shown, with the asymptotic value $\xi^{-1} = -2 \ln x$ shown as a straight line for comparison. It can be seen that the estimate $R(n)$ only approaches its asymptotic value very slowly. The finite lattice results follow the bulk limit for some distance, and then drop suddenly to zero as n approaches $M/2$, where symmetry demands that the correlation function flattens out. Thus it requires a lattice of 64 sites or bigger to see anything like the true correlation length, even at $x = 0.7$. At $x = 0.9$, 128 sites or more are required.

The situation may be improved somewhat by taking account of the expected corrections to the asymptotic behaviour. From equation (43), we expect that

$$R(n) \underset{n \rightarrow \infty}{\sim} 2 \ln \left(\frac{n+1}{n} \right) - 2 \ln x \underset{n \rightarrow \infty}{\sim} \frac{2}{n} - 2 \ln x, \quad (46)$$

so that by plotting $R(n)$ against $1/n$ one should be able to perform a sensible extrapolation to the bulk limit. Fig. 2 shows such a plot for the case $x = 0.7$. It can be seen that one could make an accurate linear extrapolation to the bulk limit, for $M = 64$, but for $M = 32$ one would only be accurate to about 10%. It requires rather large lattice sizes to get an accurate correlation length for this model.

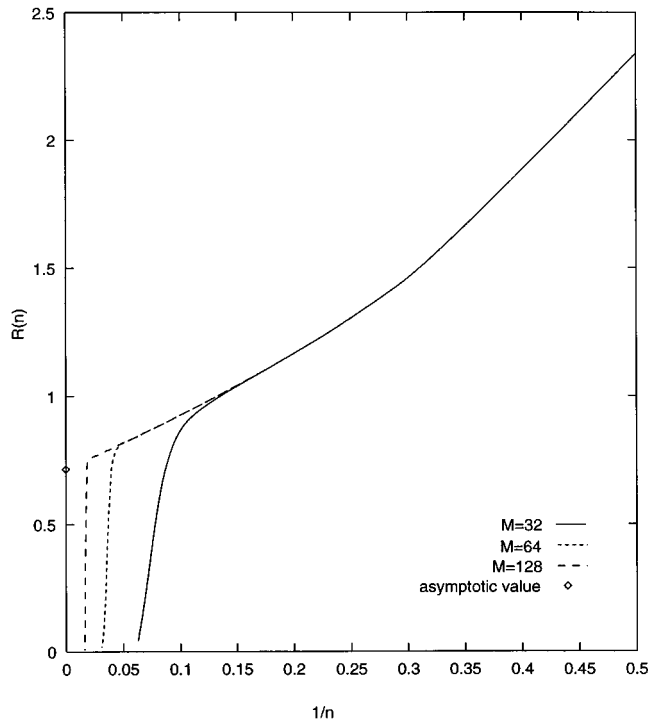


Fig. 2. The ratio $R(n)$ as a function of $1/n$ for lattice sizes 32, 64 and 128 at $x = 0.7$. The asymptotic value is shown as a diamond on the axis.

Régime $x > 1$

Corresponding results apply in the ‘low-temperature’ régime $x > 1$. In this region, there is a spontaneous magnetisation in the x direction, which has been calculated by McCoy (1968):

$$M_x = \left(1 - \frac{1}{x^2}\right)^{\frac{1}{8}}, \quad (47)$$

corresponding to the critical index $\beta = \frac{1}{8}$. In the bulk limit $M \rightarrow \infty$, n finite, the function $G(n)$ becomes as before

$$G(n) \xrightarrow{M \rightarrow \infty} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq e^{iqn} \left(\frac{1 + xe^{iq}}{1 + xe^{-iq}} \right)^{\frac{1}{2}}. \quad (48)$$

Contracting the contour onto the cut from $z = e^{iq} = 0$ to $z = -1/x$, and expanding about $z = -1/x$, one finds

$$G(n) \rightarrow \frac{(-1)^n}{\pi x^n} \left[(x^2 - 1)^{-1/2} B\left(n + \frac{1}{2}, \frac{3}{2}\right) - \frac{1}{2(x^2 - 1)^{\frac{3}{2}}} B\left(n + \frac{1}{2}, \frac{5}{2}\right) + \dots \right] \quad (49)$$

and similarly

$$G(-n) \rightarrow \frac{(-1)^{n-1}}{\pi x^n} \left[(x^2 - 1)^{\frac{1}{2}} B\left(n - \frac{1}{2}, \frac{1}{2}\right) + \dots \right] \quad (50)$$

and hence

$$\rho_c^z(n) \underset{n \rightarrow \infty}{\sim} \frac{x^{-2n}}{2\pi n^2} [1 + O(n^{-1})] \quad (51)$$

$$\sim \frac{1}{2\pi n^2} e^{-2(x-1)n}, \quad (x \rightarrow 1+) \quad (52)$$

which again agrees with the ansatz (41), with $v = 2$. For the other correlation functions, we find (Barouch and McCoy 1971)

$$\rho^x(n) \underset{n \rightarrow \infty}{\sim} M_x^2 + \frac{x^{-2n-2}}{2\pi n^2} \left(1 - \frac{1}{x^2}\right)^{-7/4} [1 + O(n^{-1})], \quad (53)$$

$$\rho^y(n) \underset{n \rightarrow \infty}{\sim} \frac{x^{-2n}}{2\pi n^3} \left(1 - \frac{1}{x^2}\right)^{-3/4} [1 + O(n^{-1})]. \quad (54)$$

All these correlation functions decay with the same exponent in this region, controlled by the energy gap to a 'kink-antikink' state in the vacuum sector. None of the local spin operators can excite a lower energy, single kink state, by reason of topological considerations.

3. Timelike Correlation Functions

Information about the energy spectrum can also be obtained from the timelike correlation functions, although it is not possible to exploit this possibility with the present algorithm, where no time appears. Timelike correlation functions for the transverse Ising model have been discussed by Niemeijer (1967), McCoy *et al.* (1971) and Lajzerowicz and Pfeuty (1975). Define the space-time correlation functions

$$\rho_{vv}(n, t) = \langle 0 | e^{iHt} \sigma_v(m) e^{-iHt} \sigma_v(m+n) | 0 \rangle, \quad (55)$$

where $v = x, y, z$ (this definition differs by a factor of 4 from previous ones—see Niemeijer 1967, McCoy *et al.* 1971 and Lajzerowicz and Pfeuty 1975); and consider the limit n fixed, imaginary time $\tau = it \rightarrow \infty$. The most interesting régime for our purpose is the 'high-temperature' régime $x < 1$. There, the results of McCoy *et al.* (1971) for the transverse correlation function translate to

$$\rho_{vv}(n, -i\tau) \underset{n \text{ fixed}}{\sim} c_v \tau^{-1/2} \exp[-2(1-x)\tau] \quad (56)$$

for $v = x, y$, where c_v is a constant depending on x . These results should be compared with the form obtained by inserting a complete set of eigenstates of H :

$$\rho_{vv}(n, -i\tau) = \sum_k \langle 0 | \sigma_v(m) | k \rangle \langle k | \sigma_v(m+n) | 0 \rangle e^{-(E_k - E_0)\tau}. \quad (57)$$

Thus the exponent in equation (56) corresponds to the mass gap ($E_1 - E_0$) of equation (8) as expected; but the exponential is modulated by an extra factor of $\tau^{-1/2}$, which can be viewed as arising from an integration over the continuum of different momentum states above the threshold. Once again, this extra power-law term will make it more difficult to extract an accurate phenomenological value for the energy gap from numerical estimates of the timelike correlation function. One will need to enhance or select out by some means the contribution to the signal coming from the lowest, zero momentum state.

4. Monte Carlo Methods

The Green's Function Monte Carlo (GFMC) method is used to simulate the Schrödinger equation for many-body systems (Ceperley and Kalos 1979; Nightingale and Blöte 1986; Ceperley 1997). The wavefunction is represented by a weighted distribution of 'random walkers' in configuration space: after many iterations of a stochastic process simulating the Schrödinger equation, the walkers approach an equilibrium distribution representing the ground state.

We implement the 'forward-walking' algorithm (Kalos 1966; Liu *et al.* 1974; Whitlock *et al.* 1979) in conjunction with the GFMC method, in order to calculate expectation values in the ground state. This technique was first used for a lattice

spin model by Runge (1992*a*, 1992*b*) in the case of the Heisenberg model. For completeness, let us summarise these methods.

The Hamiltonian H is used as the projection operator for this discrete system, after a rearrangement so as to make the ground state the dominant eigenvector. The GFMC method then produces the dominant eigenvector and eigenvalue by forming a sequence of unnormalised approximations to the exact eigenvector $|\psi_0\rangle$. Define

$$K = E_{\text{cut}} - H, \quad (58)$$

where E_{cut} is a suitably large energy cutoff so that K , the new Hamiltonian, is positive definite. The initial trial wavefunction is defined as $|\psi_T\rangle$. Each iteration corresponds to a multiplication by K . After L iterations

$$K^L |\psi_T\rangle \underset{L \rightarrow \infty}{\sim} \text{const } E_0^L |\psi_0\rangle, \quad (59)$$

where E_0 , the ground state energy, is the dominant eigenvalue of K . Hence repeated iterations project out the ground state $|\psi_0\rangle$.

Working in the spin basis $|S\rangle$, where $S = (S_1^z, \dots, S_N^z)$ is the spin configuration of the system, we define a walker as a spin and weight pair (S_i, w_i) (Nightingale and Blöte 1986). The MC algorithm simulates the Hamiltonian matrix elements $K(S', S) = \langle S' | K | S \rangle$ as transition probabilities, and the ground state wavefunction $\psi_T(S) = \langle S | \psi_T \rangle$ as the steady-state distribution of walkers, weighted by $\{w_i\}$.

The eigenvector $|\psi_0\rangle$ expands as

$$|\psi_0\rangle = \sum_i a_i |S_i\rangle, \quad (60)$$

where the amplitudes a_i obey the Schrödinger equation

$$a_k = \frac{1}{E_0} \sum_i K_{ki} a_i. \quad (61)$$

In the GFMC, the wavefunction is represented at the L^{th} iteration by

$$|\psi_0^{(L)}\rangle = \sum_i w_i^{(L)} |S_i\rangle, \quad (62)$$

where $w_i^{(L)}$ is the weight of the i th walker at iteration L . The walkers $(S_i, w_i^{(L)})$ evolve to $(S_{i'}, w_{i'}^{(L+1)})$, according to

$$w_{i'}^{(L+1)} = \sum_{S_i} \left[\frac{K(S_{i'}, S_i) w_i^{(L)}}{\mathbf{S}^{(L)}} \right] \quad (63)$$

simulating equation (61), where the 'score' $\mathbf{S}^{(L)}$ is an approximation to the eigenvalue E_0 . The score is updated after each iteration according to the following rule:

$$\mathbf{S}^{(L+1)} = \frac{W^{(L+1)}}{W^{(L)}} \mathbf{S}^{(L)}, \quad (64)$$

where $W^{(L)}$ is the 'ensemble' size or total weight

$$W^{(L)} = \sum_i w_i^{(L)}. \quad (65)$$

In order to contain the number of walkers to a manageable size and to maintain statistical accuracy, the new weights are adjusted by a stochastic 'branching' process at each iteration, represented by the square brackets in equation (63). When a weight w_i exceeds (say) 2, the walker is split into two identical copies, each with $\frac{1}{2}$ the original weight. Conversely, walkers with weights less than (say) $\frac{1}{2}$ are combined in a stochastic fashion such as to leave the total weight unchanged (Runge 1992a, 1992b).

After many iterations, the walkers approach a steady-state distribution, and the score reaches an equilibrium value, which can be averaged to give an estimate of the ground-state energy (the 'normalisation' estimate).

It is well known that to obtain good accuracy from this sort of approach one must use 'variational guidance' to herd the ensemble towards the most important regions of configuration space (Ceperley and Kalos 1979). This is achieved by means of a similarity transformation:

$$\tilde{K}(S', S) = \psi_T(S') K(S', S) \psi_T^{-1}(S), \quad (66)$$

$$\tilde{\psi}_0(S) = \psi_T(S) \psi_0(S), \quad (67)$$

where $\psi_T(S)$ is some variational estimate of the ground state wavefunction. If $\psi_T(S)$ were actually identical to $\psi_0(S)$, one can show that the GFMC procedure gives the energy E_0 exactly, with no error.

Forward Walking

The forward-walking method is an unbiased technique for estimating expectation values, based on the following equation for an operator Q :

$$\langle Q \rangle = \frac{\langle \psi_0 | Q | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \quad (68)$$

$$\underset{J \rightarrow \infty}{\sim} \frac{\langle \psi_T | K^J Q | \psi_0 \rangle}{\langle \psi_T | K^J | \psi_0 \rangle} \quad (69)$$

$$= \frac{\sum \tilde{K}(S_J, S_{J-1}) \dots \tilde{K}(S_2, S_1) Q(S_1) \tilde{\psi}_0(S_1)}{\sum \tilde{K}(S_J, S_{J-1}) \dots \tilde{K}(S_2, S_1) \tilde{\psi}_0(S_1)}, \quad (70)$$

where for simplicity we have assumed that the operator Q is diagonal in the basis of spins S .

This equation is implemented by (Kalos 1966; Liu *et al.* 1974; Whitlock *et al.* 1979):

- (i) recording the value $Q(S_i)$ for each walker ('ancestor') at the beginning of a measurement;
- (ii) propagating the ensemble as normal for J iterations, keeping a record of the 'ancestor' of each walker in the current population; and
- (iii) taking the weighted average of the $Q(S_i)$ with respect to the weights of the descendants of S_i after the J iterations.

The drawback to this procedure is that after a large number of iterations J many of the 'ancestors' will die out, leaving no descendants, which leads to a progressive loss of statistical accuracy. Thus, it is even more crucial in this connection to use a good guiding wavefunction $\psi_T(S)$ so as to minimise 'branching'.

5. Results

The Green's function method has been used to calculate the ground-state energy, the magnetisation M_z and the longitudinal correlation function $\rho^z(n)$ for lattice sizes of up to 32 sites with periodic boundary conditions. These are technically the easiest quantities to calculate in the 'high temperature' representation where σ^z is diagonal. The guiding wavefunction was taken to be of the simple form

$$\psi_T(s) = \exp \left(-c \sum_m \sigma_z(m) \right). \quad (71)$$

One could easily find more complicated and more accurate guiding wavefunctions, but since our purpose is to test the algorithms rather than to obtain accurate results for the Ising model *per se*, there seemed to be no point in using unnecessary refinements. For a review see Runge (1992a). At each coupling x , the variational parameter c was adjusted to minimise the error by a series of trial runs. Production runs typically employed an ensemble size of 2000 walkers for 10000 iterations. A certain number of the initial iterations (between 1000 and 4000) were discarded to allow for equilibration, and the results were averaged over blocks of up to 64 iterations before estimating the error to minimise correlations between measurements.

Table 1. Ground state energy per site ϵ_0 at $x = 1.0$, for lattice sizes 8, 16, 32. Monte Carlo estimates with $c = 0.3$ compared to exact results

Lattice size	8	16	32
Monte Carlo estimate	$-0.2816(1)$	$-0.2754(1)$	$-0.2737(1)$
Exact	-0.281458	-0.275287	-0.273751

Ground State Energy

The results for the ground state energy per site ϵ_0 at the critical point $x = 1$ are shown in Table 1, and compared with the exact results from equation (2).

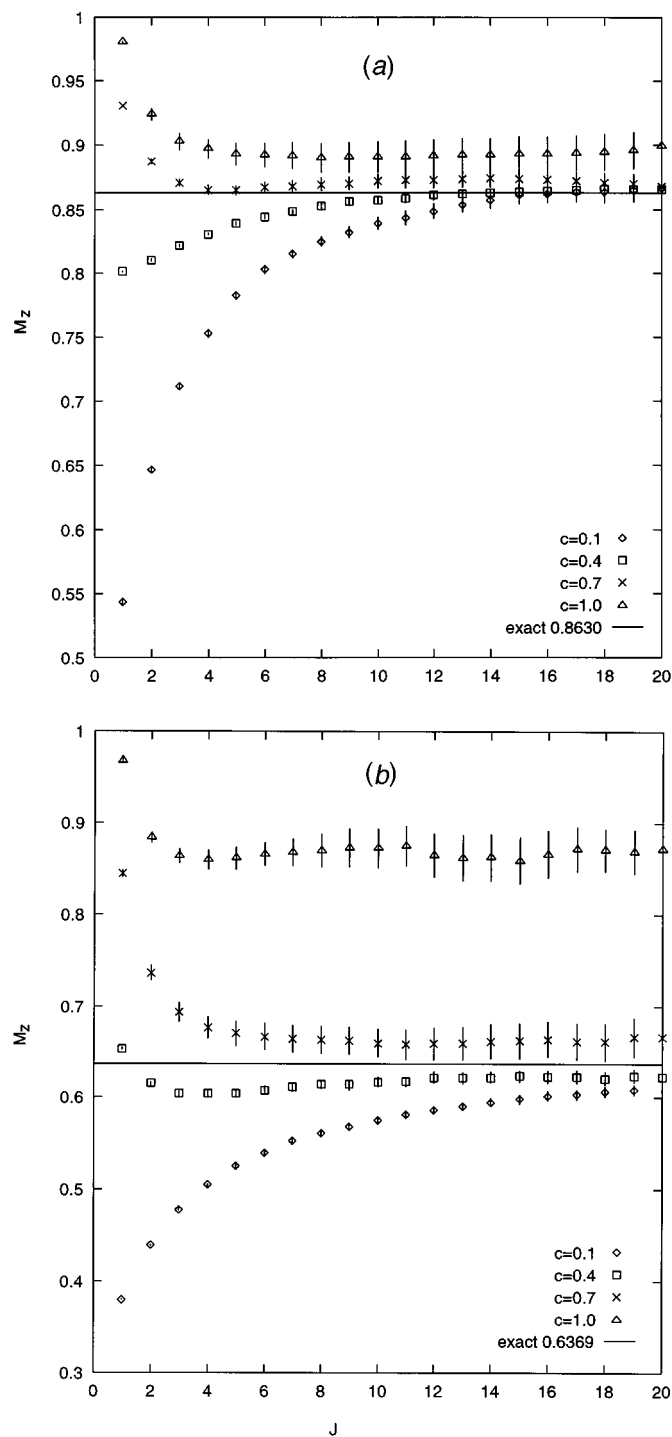


Fig. 3. Estimates of M_z as a function of J , the number of forward walking iterations, for lattice size $M = 32$ at: (a) $x = 0.7$ and (b) $x = 1.0$. The horizontal line indicates the exact value.

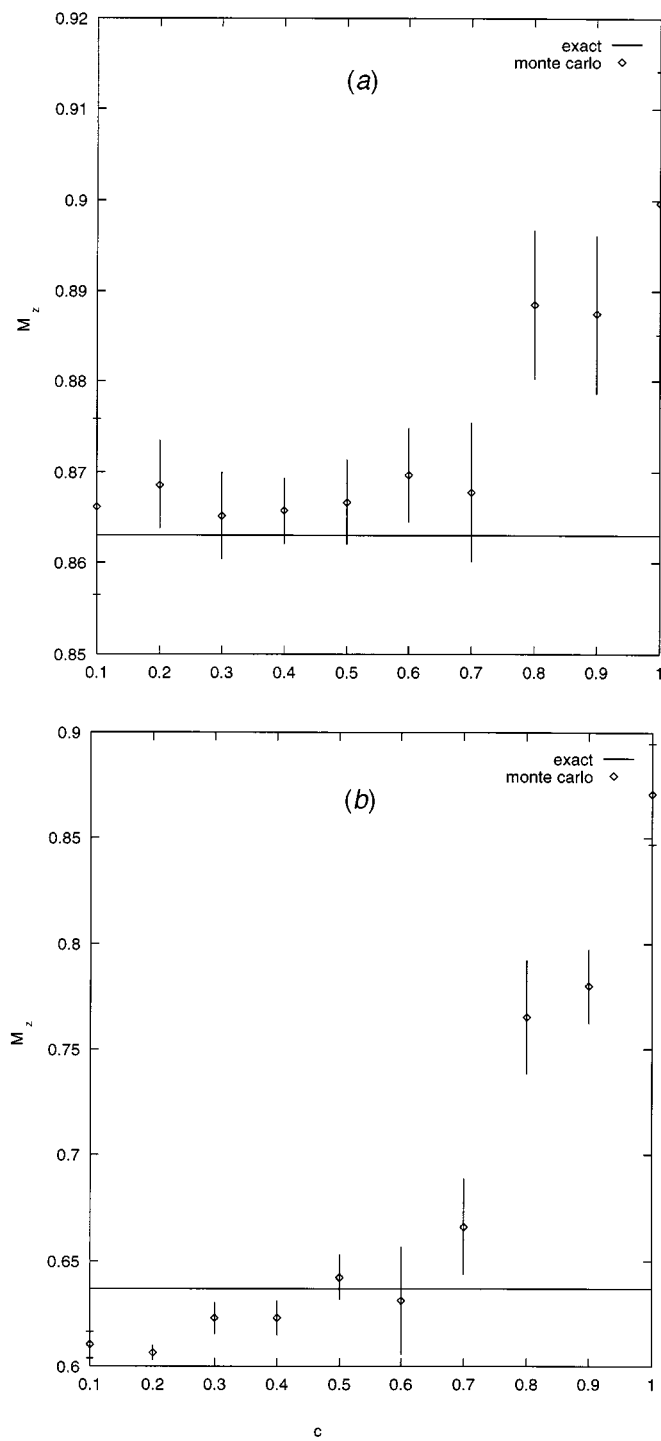


Fig. 4. Monte Carlo estimates of the magnetisation M_z as a function of the variational parameter c for lattice size 32 at: (a) $x = 0.7$ and (b) $x = 1.0$.

For all three lattice sizes 8, 16 and 32 the best result for the ground state energy occurs at $c \approx 0.3$. It can be seen that the errors in the Monte Carlo estimates are of order 0.04%: away from the critical point they are substantially less.

Magnetisation

As a first example of an expectation value estimated by the 'forward-walking' technique, we consider the magnetisation in the z -direction M_z . Measurements were started every 250 iterations, and the ancestor weights were tracked for up to twenty 'forward-walking' iterations, J , each time; the results of the iterations were then block-averaged in the same way as the ground state energy.

Fig. 3a shows the estimated value of M_z as a function of J , the number of forward-walk iterations, for various values of the variational parameter c , at a coupling of $x = 0.7$. It can be seen that the results converge to the correct value, within errors, after 10–20 iterations, for a range of different values of c . The convergence appears to be best for an optimal value of $c \approx 0.5$. If c is chosen too large, however, then an incorrect estimate may be obtained, as in the case $c = 1.0$.

Fig. 3b shows a similar graph at the critical point $x = 1.0$. It can be seen in this case that the estimates take a good deal longer to relax to their asymptotic value; and also that the results are much more sensitive to the variational parameter c . To obtain accurate results at a critical point by this technique, it is crucial to have a good trial wavefunction, and choose the variational parameter judiciously.

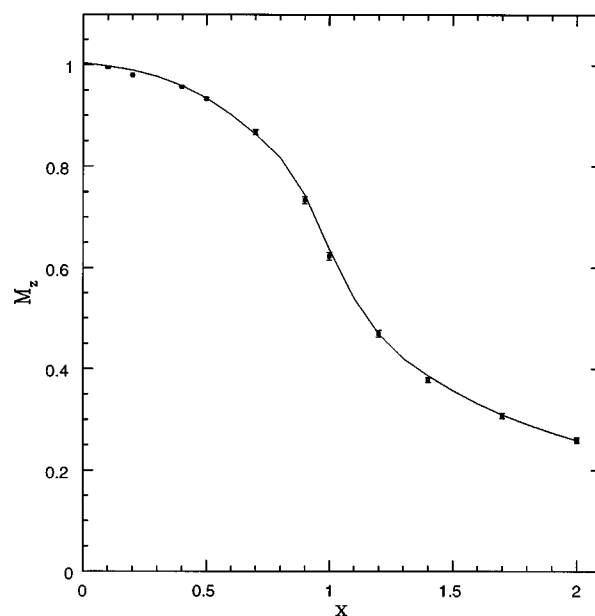


Fig. 5. Forward-walking estimates of magnetisation M_z as a function of x compared with the exact results (curve) for 32 lattice sites.

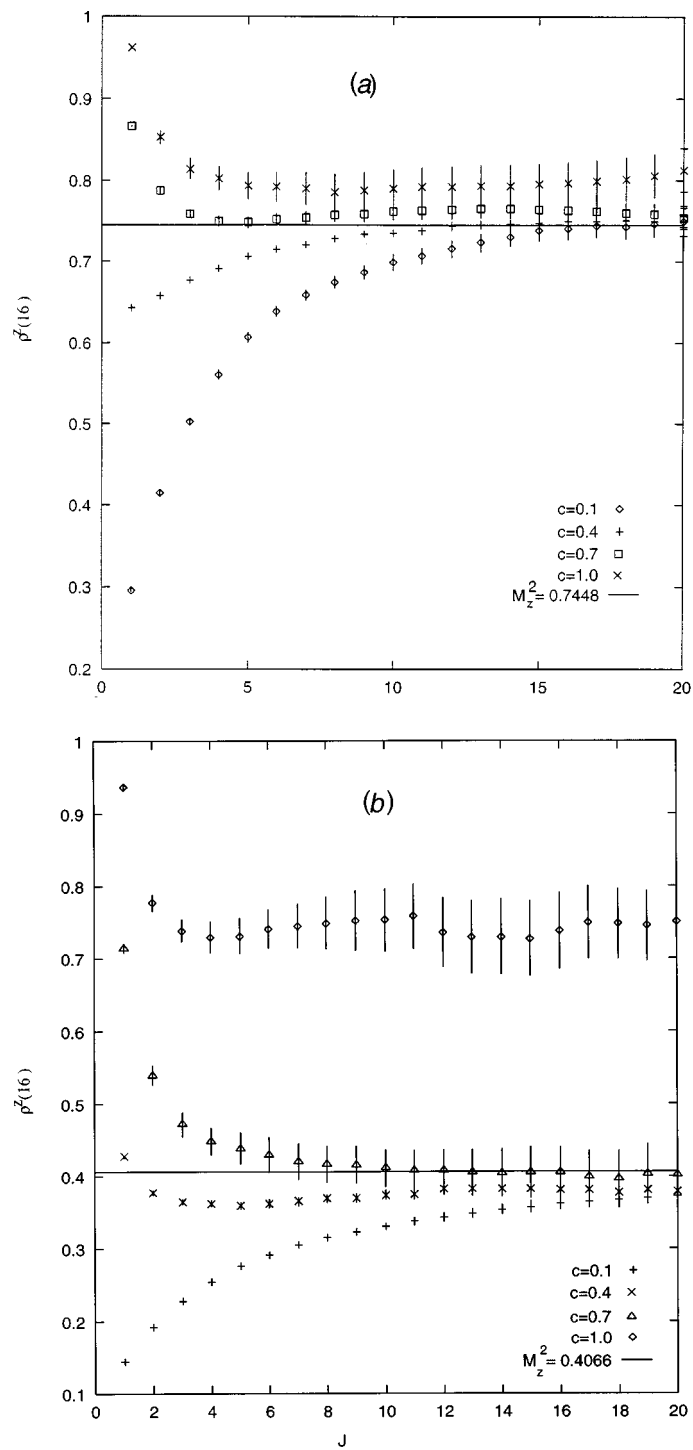


Fig. 6. Estimate of $\rho^z(16)$ on the $M = 32$ lattice, as a function of the number of forward-walking iterations J , for various values of c and for: (a) $x = 0.7$ and (b) $x = 1.0$.

In Fig. 4 the final Monte Carlo results for M_z versus the coupling parameter c are plotted at (a) $x = 0.7$ and (b) 1.0 , with the exact value (horizontal line) used as a comparison. At $x = 0.7$ (Fig. 4a), the estimates form a reasonably stable 'plateau' for $0.1 < c < 0.7$, corresponding to the correct value for $M - z$ within errors; but as c increases further towards 1.0 , the estimates drift away from the correct value. The 'best' estimate of c is obtained by choosing a value in the middle of the 'plateau' where the result for the observable are stable and the error is least; for the energy this occurs at $c = 0.5$ and for M_z it lies between $c = 0.4$ and $c = 0.5$. At $x = 1.0$ (Fig. 4b), the 'plateau' is not quite so obvious, but the estimates are reasonably stable, and cluster about the correct value, for $0.3 \leq c \leq 0.6$. The 'best' value for both the energy estimate and M_z seems to lie around $c = 0.3$.

Fig. 5 shows the final Monte Carlo estimates of M_z for the 32 site lattice as a function of x (at the best variational parameter c). It can be seen that the Monte Carlo estimates are generally in good agreement with the exact results, with the largest error 1% occurring at the critical point $x = 1.0$.

Correlation Functions

Our major interest in this study is the computation of correlation functions—more specifically, $\rho^z(n)$. These expectation values were estimated in exactly the same way as the magnetisation. Fig. 6a shows estimates of $\rho^z(16)$ on the $M = 32$ lattice at $x = 0.7$, as a function of the number of forward-walking iterations J ,

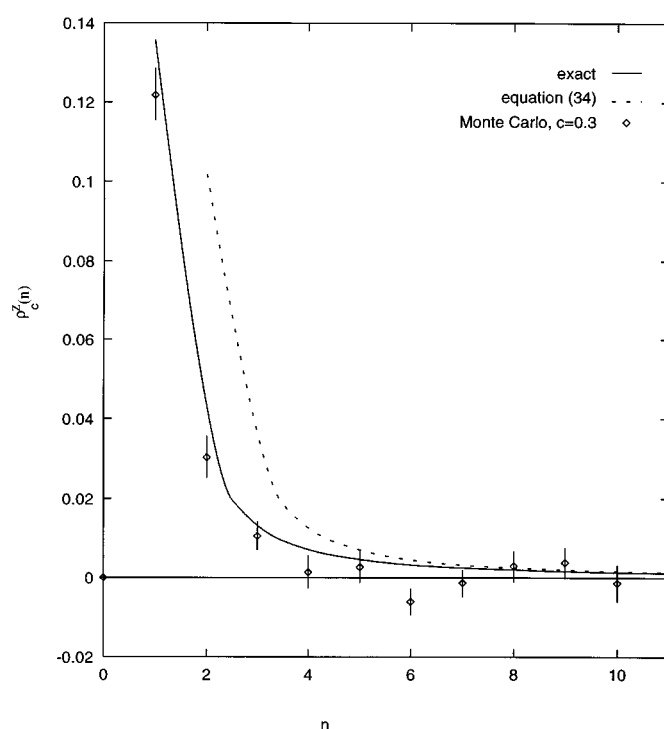


Fig. 7. Monte Carlo estimates of the connected correlation function $\rho_c^z(n)$ as a function of n for $x = 1.0$ and lattice size $M = 32$ sites. The exact result (solid curve) and asymptotic form of equation (35) (dotted curve) are shown for comparison.

for various values of c . It can be seen that the results converge just as well as for the magnetisation in Fig. 3a, and the same comments apply. The asymptotic estimates cluster around the correct value for $0.1 \leq c \leq 0.7$, but drift away as c increases further. Fig. 6b shows a similar graph at the critical point $x = 1.0$, which again looks very similar to the magnetisation results of Fig. 3b. The estimates converge at close to the true value, except for the case $c = 1.0$, where they are much too high. The conclusion seems to be that it is no more difficult to measure the absolute value of a correlation function than it is to measure a ‘local’ observable such as the magnetisation.

The snag is, of course, that the absolute value of the ‘connected’ correlation function $\rho_c^z(n)$, obtained when one subtracts off M_z^2 , dies off rapidly towards zero as n increases, and thus the relative error in $\rho_c^z(n)$ rapidly increases. Fig. 7 shows our Monte Carlo estimates of $\rho_c^z(n)$ as a function of n at $x = 1.0$ for the 32 site lattice, together with the exact result and the asymptotic form given by equation (35). It can be seen that the Monte Carlo estimates agree with the exact results within errors, but with our present crude trial-wavefunction and limited statistics, the errors are too large to obtain useful estimates beyond about $n = 4$. A good trial wavefunction and high statistics will be required, in general, to track the correlation functions at large distances.

6. Conclusions

The forward-walking Green’s Function Monte Carlo method has been used to compute expectation values such as the magnetisation M_z and the correlation function $\rho^z(n)$ for the transverse Ising model in $(1+1)D$. The algorithm successfully reproduces the exact results within 1% or better at criticality, and gives substantially better results away from the critical point. One encouraging feature is that the results for ‘non-local’ properties such as long-range correlations converge almost as rapidly as for local quantities such as the magnetisation.

As expected (Ceperley and Kalos 1979; Ceperley 1997), the results are quite sensitive to the trial wavefunction (or in this case the parameter c), particularly at the critical point. If one chooses a bad value for the parameter c , such as $c = 1$ in Fig. 6b, one can obtain quite wrong values for the expectation values. The trial wavefunction provides such a sharp cutoff in this case that it does not allow a proper sampling of the configurations with many ‘flipped’ spins. To achieve good accuracy, it is important to use a good trial wavefunction, and to optimise the variational parameters carefully. This can be done by performing a separate variational Monte Carlo calculation, or by looking for a ‘valley’ in parameter space where the ground-state energy estimate is a minimum and its variance is least. At $x = 1$, this procedure points to $c \simeq 0.3$ as optimum, far from $c = 1.0$. In most cases a ‘plateau’ region is observed, where the estimates are reasonably stable against the variational parameter, and agree with the exact results within errors. Thus we conclude that the method should be suitable for use in calculating correlation functions for more complicated and more interesting lattice models.

We have also spent some time analysing the exact results for the model. It has been shown that in the neighbourhood of the critical point the correlation functions have the exponential behaviour in space and (imaginary) time which

is expected of the corresponding continuum field theory, and that the mass gaps can in principle be measured from the exponents. It was also seen, however, that the presence of extra power-behaved terms modulating the exponentials is liable to complicate the process of estimating the exponents. A method of plotting the data was discussed which allows one to overcome this problem to some extent—see Fig. 2.

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