Test for random number generators: Schwinger-Dyson equations for the Ising model

H. G. Ballesteros* and V. Martín-Mayor†
Departamento de Física Teórica I, Universidad Complutense de Madrid, 28040 Madrid, Spain
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We use a set of Schwinger-Dyson equations for the Ising model to check several random number generators. For the model in two and three dimensions, it is shown that the equations are sensitive tests of bias originating with the random numbers. The method is almost costless in computer time when added to any simulation. [S1063-651X(98)05411-7]

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I. INTRODUCTION

Among the sources of systematic error in Monte Carlo (MC) simulations, the most frightening is the lack of randomness in the pseudorandom number generator (PRNG). Indeed, in a modern MC simulation as many as 10^{13} random numbers may be generated [1]. This is as long as the longest test of random numbers we have heard of [2]. Therefore, a PRNG needs to be fast and thus not too sophisticated, but it also should not bias the simulation results. Shift-register PRNG's [3] have become very popular, due to their speed, but they have been shown to be unreliable for some applications [4]. The study of the trustworthiness of a PRNG is quite difficult as the answer is problem-dependent, algorithm-dependent, and (most important) precision-dependent. For instance, in Ref. [5] some commonly used shift-register PRNG's were shown to yield incorrect results for the two-dimensional Ising model simulated with the Wolff's single-cluster algorithm [6]. Of course, this failure is related to one's statistical accuracy (all the generators in Ref. [5] would be ''correct'' with 5% errors). In particular, the R250 shift-register PRNG was found to be very dangerous for a single-cluster update, but safe for use with the Metropolis algorithm. Not long after that, R250 was shown to fail in the Metropolis update of the Blume-Capel model for some lattice sizes [7]. Another example of the difficulty in certifying PRNG's can be found in Ref. [8]. There, the standard Cray PRNG (usually called RANF) is shown to be ''very good'' in the author's own wording. This means that the longest run did not find bias in a two-dimensional Ising model simulation, where comparison with the exact solution was possible [9]. Nevertheless, it has produced wrong results in a U(1) lattice gauge-theory simulation [10]. Moreover, it is fairly common for one's simulation to be, itself, the longest run ever carried out for this particular problem (otherwise, why bother doing it?). Unless independent, algorithmically different simulations are performed, it is clear that one's result will not be yet *established*. Further confidence can be obtained if sensitive consistency tests are also carried out. In this paper, we want to show that Schwinger-Dyson identities may be useful in this respect, especially when no exact solution is at hand. Let us finally mention that the investigation of the reasons for PRNG-induced bias is interesting in itself [11], but it has not yet reached predictive power (one wants to know *before* carrying out the simulation).

II. THE EQUATIONS

Generally speaking, Schwinger-Dyson equations are relations of the type

$$0=\left\langle \frac{\delta O}{\delta\phi(x)}\right\rangle - \left\langle O\frac{\delta H}{\delta\phi(x)}\right\rangle, \tag{1}$$

where O is an arbitrary operator and H is the Hamiltonian [notice, however, that for Eq. (1) not to be a trivial $0=0$ statement, O should be an odd operator if H is symmetric under the $\phi\to-\phi$ transformation]. The problem is that the longest MC runs are usually done in discrete spin models, for which there are no continuous variables. Nevertheless, for spin models the measure usually has a Z_2 symmetry, which allows us to obtain equations analogous to Eq. (1). As an example, let us consider the Ising model on the cubic lattice, with nearest-neighbors interaction. The Hamiltonian is

$$H=-\beta\sum_{\langle i,j\rangle}\sigma_i\sigma_j, \tag{2}$$

where σ are the usual Z_2 spin variables. Let us call S_i the sum of the spins coupled with spin σ_i. The self-evident relation

$$\sum_{\sigma=-1,1} f(\sigma)=\sum_{\sigma=-1,1} f(-\sigma),$$

yields for any observable depending on the spin σ_i (and possibly also on others), $O(\sigma_i;\dots)$, the following relation:

$$\langle O(\sigma_i;\cdots)\rangle=\langle O(-\sigma_i;\cdots)e^{-2\beta\sigma_i S_i}\rangle. \tag{3}$$

In particular, one gets

$$1=\langle e^{-2\beta\sigma_i S_i}\rangle, \tag{4}$$

$$\langle\sigma_i\sigma_j\rangle=-\langle\sigma_i\sigma_j e^{-2\beta\sigma_i S_i}\rangle+2\delta_{ij}, \tag{5}$$

where δ_{ij} is the Kronecker symbol. In order to improve statistics, it is useful to sum Eq. (4) for all the lattice sites (the lattice size being L, its volume is $V=L^D$). One obtains

*Electronic address: hector@lattice.fis.ucm.es
†Electronic address: victor@lattice.fis.ucm.es

$$1=\left\langle \frac{1}{V}\sum_i e^{-2\beta\sigma_i S_i}\right\rangle. \tag{6}$$

Summing to the nearest neighbors in Eq. (5), we obtain an expression which is very useful in MC renormalization group investigations of the dynamics of the Poliakov loop in lattice gauge theories [12]:

$$0=\left\langle \frac{1}{V}\sum_i \sigma_i S_i(1+e^{-2\beta\sigma_i S_i})\right\rangle. \tag{7}$$

It is trivial to generalize Eq. (7) when more couplings are included in the Hamiltonian, as needed in a MC renormalization group study.

In addition, a nonlocal identity is obtained from Eq. (5) summing to all i and j:

$$0=-\frac{2}{V}+\left\langle \frac{1}{V^2}\sum_{i,j} \sigma_i\sigma_j(1+e^{-2\beta\sigma_i S_i})\right\rangle. \tag{8}$$

At this point, it is natural to ask if the right-hand sides of Eqs. (6), (7), and (8) can be measured with reasonable statistical accuracy. We shall see that the answer is positive. Then the next natural question to ask is if a PRNG-inducing bias also spoils the fulfillment of these equations. We shall find a positive answer only for Eqs. (6) and (7).

Finally, let us mention that the Z_2 symmetry is embedded in the symmetry of many other models, therefore Eqs. (6), (7), and (8) hold as they are for O(N) spin models, or, with trivial modifications, for SU($2N$) lattice gauge theories.

III. NUMERICAL RESULTS

We have studied the Ising model (with periodic boundary conditions) in two and three dimensions at their critical points. Three update methods have been considered: Metropolis [13], the Swendsen-Wang cluster method [14], and Wolff's single-cluster (SC) [6]. For each update, we have employed three PRNG's. One has been the problematic [5] R250:

$$X_n^{\mathrm{R250}}=(X_{n-103}^{\mathrm{R250}}+X_{n-250}^{\mathrm{R250}}) \mod 2^{32}. \tag{9}$$

The second has been the Parisi-Rapuano (PR) PRNG [4], which has been found not quite correct in four-dimensional site percolation [1]:

$$X_n^{\mathrm{PR}}=Y_n \ \mathrm{xor}\ Y_{n-61}, \tag{10}$$

where

$$Y_n=(Y_{n-24}+Y_{n-55}) \mod 2^{32}.$$

Our last generator is defined with the help of a congruential generator:

$$Z_{n+1}=(16807Z_n) \mod(2^{31}-1).$$

Then, the Parisi-Rapuano-congruential (PRC) PRNG [1] is defined as

$$X_n^{\mathrm{PRC}}=(X_n^{\mathrm{PR}}+2Z_n) \mod 2^{32}. \tag{11}$$

Our statistics have been the following. In two dimensions we have considered a $L=16$ lattice. We have simulated at the exact critical point up to 6 digits:

$$\beta_c=0.440687.$$

We have measured every 20 Metropolis sweeps or 20 single clusters, performing 8×10^7 Metropolis full-lattice sweeps, and updating 4×10^7 clusters. For the Swendsen-Wang algorithm, we measured every 5 sweeps, and generated the clusters 4×10^7 times.

In three dimensions, the critical coupling is known with great accuracy [15]. We have simulated at

$$\beta=0.221654.$$

As shown in Ref. [7], it might happen that the bias only appears for some lattice sizes. Therefore, we have studied $L=16$ and 24 lattices. For Metropolis or single-cluster, we measure every 10 sweeps. We perform 10^7 Metropolis sweeps, and generate 10^7 clusters. In the Swendsen-Wang

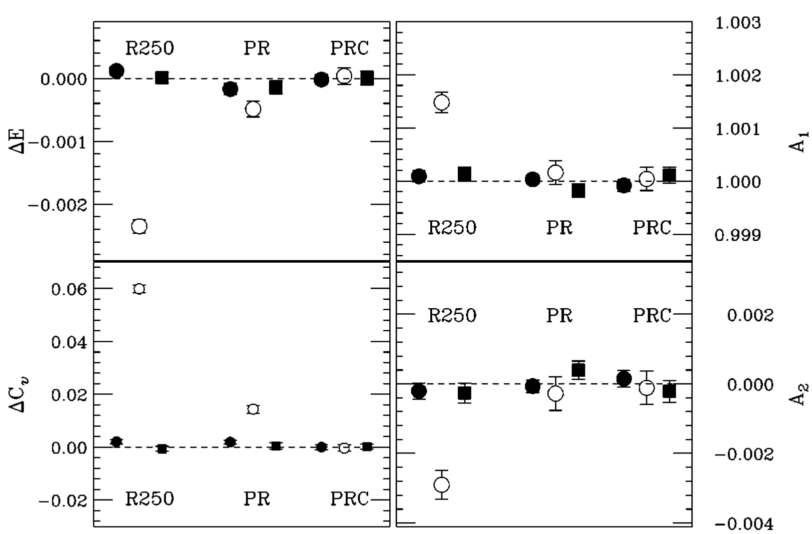

FIG. 1. Difference with the exact results for the energy and the specific heat in a 16^2 lattice. We also plot A_1 and A_2. Full circles correspond to the Swendsen-Wang update, open circles to single cluster and squares are from the Metropolis update.

case, we measure every 4 sweeps, generating the clusters 4×10^6 times. We have found quite clear results for the different simulations, except for the single-cluster update of the 16^2 and 16^3 lattices, with PR as PRNG. We have found it convenient to extend these two simulations, although this is, in principle, a dangerous procedure. Of course, one cannot proceed with the run until the results ''look nice,'' since this would bias the results. To avoid subjective decisions, we have fixed *a priori* the total (much longer than the initial) simulation time: these two simulations were 40 times longer than the others. In this way, error bars shrink enough to distinguish between a large statistical fluctuation and a systematic error.

Before presenting our results, a word of caution is in order. We have carried out 27 independent simulations (3 lattices×3 PRNG×3 updates), so, the number of expected data points which are more than one standard deviation away is uncomfortably large. Specifically, one can easily estimate that the number of points that are more than 1.7 deviations away (10% probability) must be between 2 and 4. Moreover, errors are not obtained with perfect accuracy. Allowing a 10% error in the error determination, we have considered deviations larger than 3.3 error bars as a significant signal of bias (less than a 0.13% probability).

Let us first discuss our results in two dimensions. In the left-hand side of Fig. 1 we plot the deviations of the energy and the specific-heat from their exact values [9]. We find significant deviations only for the single-cluster update when using R250 and PR as PRNG's (the former is not surprising [5]). It is clear that the exact solution is the best of possible tests, but we would like to confront it with the Schwinger-Dyson test. For this, let us define the quantities:

$$A_1 = \left\langle \frac{1}{V} \sum_i e^{-2\beta\sigma_i S_i} \right\rangle_{\mathrm{MC}},$$

$$A_2 = \left\langle \frac{1}{V} \sum_i \sigma_i S_i (1 + e^{-2\beta\sigma_i S_i}) \right\rangle_{\mathrm{MC}}, \tag{12}$$

which are the right-hand sides of Eqs. (6) and (7). Unfortunately, Eq. (8) has been found to hold within errors in all cases. In the above expressions $\langle\ \rangle_{\mathrm{MC}}$ is the MC average, not the expectation value. We show our results for A_1 and A_2 in the right-hand side of Fig. 1. The only significant deviation found is in the single-cluster update with R250. This does not mean that the Schwinger-Dyson identities can be fulfilled with a biasing PRNG, as this is, of course, a matter of accuracy. In fact, performing a 40 times longer run with PR, we find

$$A_1 = 1.00024(4),$$

$$A_2 = -0.00047(8).$$

Thus, both the exact solution test and the Schwinger-Dyson identities test failed by this SC-PR combination, but the exact solution test is more sensitive in this case.

We can discuss our results more quantitatively. For small bias, it is natural to expect that its main effect can be described as a shift on the coupling, from β to $\beta' = \beta - \Delta\beta$. With this assumption, we can relate the different bias. Let ΔO be the the difference between the mean value of O obtained with some MC simulation, and its true Boltzmann average, we obtain to first order in $\Delta\beta$ [16],

$$\Delta O \approx -\frac{\partial_\beta \langle O \rangle}{4E} \Delta A_1 . \tag{13}$$

TABLE I. The bias for E, C_v, A_1, A_2, for the 16^2 lattice simulated with the SC-**R250**, SC-**PR** combinations. To be able to measure the bias in the SC-**PR** combination, we needed a much longer simulation (see text). The constancy of the ratios is a check for Eq. (13).

	ΔE	ΔC_v	ΔA_1	ΔA_2
SC-**R250**	−0.00235(11)	0.0599(14)	0.00148(19)	−0.0029(4)
SC-**PR**	−0.00057(2)	0.0115(2)	0.00024(4)	−0.00047(8)
Ratio	0.242(14)	0.192(5)	0.16(3)	0.16(4)

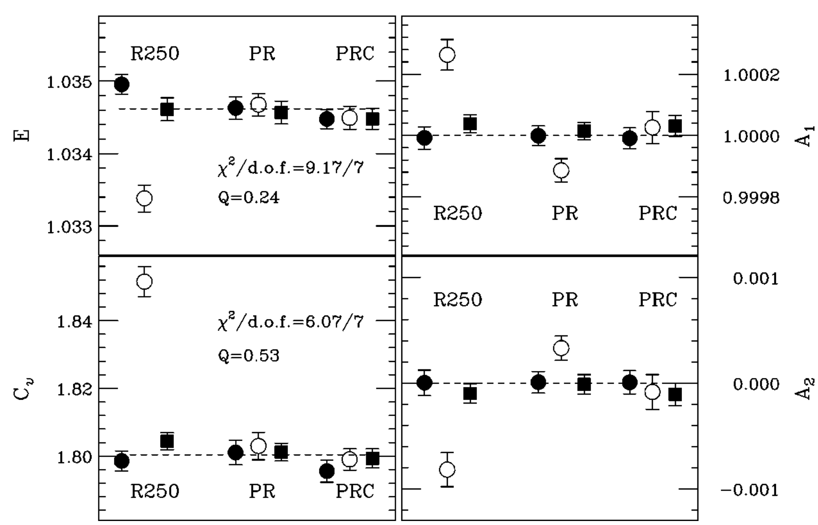

FIG. 2. Simulation results for the energy, the specific heat, A_1 and A_2, in a 16^3 lattice. Dashed lines for E and C_v are obtained from a χ^2 minimization, excluding the SC-R250 data. Q is the probability of getting a larger value of χ^2. Full circles correspond to the Swendsen-Wang update, open ones to single-cluster, and squares are from the Metropolis update.

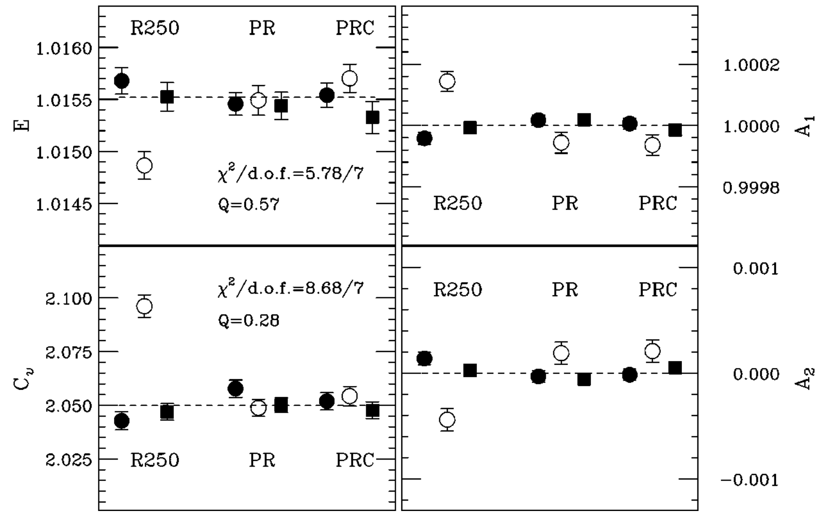

FIG. 3. Same as Fig. 2 for a 24^3 lattice.

In this way, we can understand that the bias for the energy has the opposite sign as the one for A_1 [16], and it is also opposite to the bias for the specific heat (it is well known that the maximum of the specific heat of the two-dimensional Ising model in a finite lattice is at $\beta<\beta_c$). The only evidence that we can offer for Eq. (13) is empirical, and it is shown in Table I. Nevertheless, we find the agreement quite satisfactory for such a rough calculation. Moreover, from Table I we can estimate that

$$\begin{aligned} \Delta E &\approx -1.6\Delta A_1, \\ \Delta C_v &\approx 40\Delta A_1, \end{aligned} \tag{14}$$

where the coefficient for the energy is really 1.58(19), to be compared with 1.33 from Eq. (13). Notice that if Eq. (13) could be rigorously established, it would be enough to estimate the failure in the Schwinger-Dyson test for any PRNG, to get the safe accuracy level for every observable. However, to our knowledge, such an interesting property has not been proved for any PRNG test.

For the three-dimensional case, we plot our results for the energy and the specific heat in the left-hand side of Figs. 2 and 3. In this case, we unfortunately lack an exact solution to control for the bias. However, we can study the statistical compatibility of our data. From the plot it is apparent that the SC-R250 results are biased. In the figures, we show the data with a weighted estimate of the energy and the specific heat (excluding the SC-R250 data). In fact, no further significant deviations are found. For the Schwinger-Dyson test, we find again strong signals of bias in A_1 and A_2 for the combination of R250 with single cluster. We also find worrisome deviations in the single-cluster update with PR as PRNG for $L=16$. To clarify if a bias is present in this case, we have performed a 40 times longer run. The new results are

$$A_1 = 0.999966(8),$$

$$A_2 = 0.000101(26).$$

Thus, the PR PRNG does produce biased results in combination with the single-cluster update. In this case, we cannot check Eq. (13) directly, as the deviations in the energy and specific heat for SC-PR are not large compared to the errors. Nevertheless, we can compare the bias for the SC-R250 in the 16^3 and 24^3 lattices (see Table II), which is a test of the L dependence of the linear coefficient in Eq. (13). From finite-size scaling theory, we can estimate that

$$\frac{(\Delta C_v/\Delta E)_{L=24}}{(\Delta C_v/\Delta E)_{L=16}} \approx \left(\frac{24}{16}\right)^{1/\nu} \approx 1.9\ldots, \tag{15}$$

where $\nu\approx 0.63$ is the critical exponent for the correlation length. From Table II, the above quotient can be estimated to be 1.7(5), which is certainly compatible with our prediction, but the error is so big that this is not compelling evidence for Eq. (13). Now, if we assume again Eq. (13), we obtain for the 16^3 lattice $\Delta E\approx -5\Delta A_1$ and $\Delta C_v \approx 194\Delta A_1$. From these relations, and from the estimate of $\Delta A_1^{\text{SC-PR}}$ we obtain for the bias (the statistical errors in Fig. 2 being σ_E and σ_C)

$$\begin{aligned} \Delta E^{\text{SC-PR}} &\approx 0.00015, \quad \sigma_E = 0.00019, \\ \Delta C_v^{\text{SC-PR}} &\approx 0.007, \quad \sigma_C = 0.005. \end{aligned} \tag{16}$$

Thus, it is not surprising that the bias does not show up in Fig. 2. For the 24^3 lattice we lack an accurate measure of the bias for A_1, and so we cannot obtain a bias estimate.

As a final remark, notice that the sign of the bias seems to be independent of the lattice size and the space dimension for R250. This seems to be consistent with the simple (one-dimensional) model proposed in Ref. [11]. However, in the PR case, the (much smaller) bias changes sign when going

TABLE II. Bias for E, C_v, A_1, A_2, for the 16^3 and 24^3 lattices simulated with the SC-**R250** combination. The ''correct'' value has been taken from the averaged estimate of Figs. 2 and 3. The ratios test the lattice-size dependence of the coefficients in Eq. (13).

L	ΔE	ΔC_v	ΔA_1	ΔA_2
16^3	−0.00124(19)	0.051(4)	0.00026(5)	−0.00082(16)
24^3	−0.00066(13)	0.046(5)	0.00014(3)	−0.00044(11)
Ratio	0.53(13)	0.90(12)	0.54(16)	0.54(4)

from two to three dimensions. This suggests that the reason for bias is more involved in this case.

IV. CONCLUSIONS

In this work, we have shown that some Schwinger-Dyson identities, Eqs. (6) and (7), are a sensitive test of PRNG-induced bias. Most important, they can be used when no exact solution is at hand. We have provided some empirical evidence for a simple relation between the bias induced in the different observables [our Eq. (13)]. This relation is obtained under the assumption that the main effect of the bias is to produce a shift on the coupling. It might be possible to justify this in terms of relevant and irrelevant operators, in the framework of the renormalization group. Furthermore, this suggests that an investigation along the lines of Ref. [12] could be useful to establish which new couplings are generated by the PRNG-induced bias. If this relation could be established, the Schwinger-Dyson (SD) equation test would provide an estimate on the maximum *safe* accuracy that one can get for any observable, with the given PRNG.

In three dimensions, where there is no exact solution at hand, the Schwinger-Dyson equations test has shown that the single-cluster update with the R250 and PR PRNG's produces biased results, without resource to seven more simulations. It should be noticed that the measure of the Schwinger-Dyson equations is almost computer time costless, as the number of possible exponential factors is finite, and the local energy should be measured anyway. Disk storage is not a shortcoming either, because no reweighting [17] is to be done, and the calculation can be made ''on the fly.'' They are also extremely helpful for code debugging. So, we believe Schwinger-Dyson equations to be very useful tools, which can be easily measured in almost every circumstance.

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