Comment on a Monte Carlo test of theories for the planar model, the F model, and related systems

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The numerical method of Shugard, Weeks, and Gilmer is shown to contain systematic errors that prevent it from testing theories of planar and roughening models.

Shugard, Weeks, and Gilmer[1] (SWG) have proposed a Monte Carlo (MC) test of theories for planar and roughening models. Their method is based on fitting MC data for roughening-model correlation functions to the expected logarithmic divergence[2,3]

$$G(r) = \langle (h_0 - h_r)^2 \rangle \rightarrow B(\ln r + C) \ . \quad (1)$$

Since every two-dimensional XY model is related to some roughening model by an exact duality transformation[4,5] and it had been previously shown that MC simulations in the roughening representation have advantages over MC simulations in the XY representation for calculating properties of XY models,[6,7] SWG also applied their method to XY models.

To establish the accuracy and reliability of their method, SWG tested it on the body-centered solid-on-solid (BCSOS) model [introduced by van Beijeren[8] and called the F-model SOS (FSOS) by SWG] at $T = 2T_R$, where $B = 4/\pi^2$,[9] and $T = T_R$, where $B = 2/\pi^2$,[10] in agreement with the Kosterlitz-Thouless (KT) theory.[11-14] They claimed that the agreement was "excellent"[1] and that their procedure was "much less subject to error from statistical fluctuations than are methods which examine divergences in such quantities as the interface width."[1]

I have repeated their calculations and come to different conclusions. The SWG method is subject to *larger* statistical errors than the older methods and, in addition, contains systematic errors that affect the value of B by as much as 20%.

SWG used "60 × 60 lattices" (which actually contain 7200 sites) for their MC simulations and their stated procedure was to "assume that the curves have reached their asymptotic value by 7 units and use the region from 7 to 12 to determine the parameters."[1]

In repeating SWG's calculation for the BCSOS model at $T = 2T_R$, I averaged over 8×10^4 Monte Carlo steps per site (MCS/S) (compared with their 2.22×10^4 MCS/S) at intervals of 50 MCS/S (SWG: 278 MCS/S) after an equilibration run of 2×10^4 MCS/S (SWG: 5.6×10^3 MCS/S). Errors were determined by the usual method of dividing the runs into groups, calculating the properties of interest for each group, and looking at the spread of values as a function of the size of the group. It is worth noting that the error in $G(r)$ for fixed r (which I found to be in agreement with SWG) does not provide a reliable indication of the error in the slope, B, due to the strong correlations between the estimates for $G(r)$ and $G(r')$. Consequently, the errors for each estimate of B in Eq. (1) must be calculated separately.

It turned out that it was not necessary to use all the data between 7 and 12 together (as SWG did) to obtain a clear result. We can also simply use two successive values of $G(r)$ to define

$$B(r) = \frac{G(r+\frac{1}{2}) - G(r-\frac{1}{2})}{\ln(r+\frac{1}{2}) - \ln(r-\frac{1}{2})} \ . \quad (2)$$

This quantity is divided by its expected asymptotic value of $4/\pi^2$ and plotted vs r in Fig. 1.

If $G(r)$ really had reached and maintained its asymptotic behavior for $7 \leq r \leq 12$, $B(r)/(4/\pi^2)$ would have had a constant value of unity in Fig. 1. The fact that it shows a decrease, with the deviation reaching 10% for $r = 11.5$, is due to a well-known finite-size effect. Because of the periodic boundary conditions, $G(r)$ for a system with linear dimensions N must also be periodic and symmetric: $G(N-r) = G(r)$. This means that the slope at $r = \frac{1}{2}N$ is zero. Consequently, $B(r) \rightarrow 0$ as $r \rightarrow \frac{1}{2}N = 30$ and it is not surprising that the decrease is already substantial at $r \approx 12$.

SWG did not actually fit B to the MC data, preferring to set B to the expected value and to fit the additive constant C. Since the curves are fairly flat, this gives the appearance of excellent agreement. My data looks the same as theirs if I plot $G(r)$ vs r. However, fitting B and C to all MC data between 7 and 12, I find a calculated value of B that is 6.0(±1.5)% *below* the exact value due to the finite-size effect.

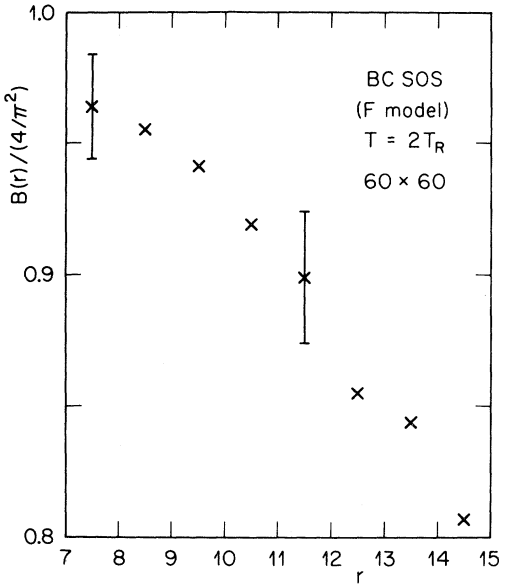

FIG. 1. MC data for $B(r)=\delta G(r)/\delta \ln r$ as a function of r for the BCSOS model on a 60×60 lattice at $T=2T_R$.

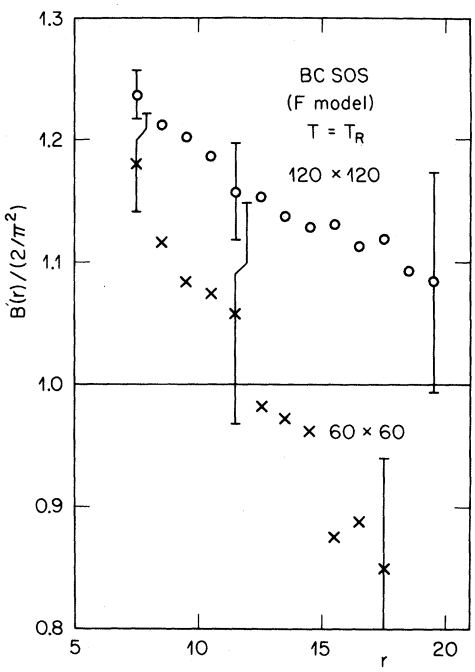

FIG. 2. Same as Fig. 1 for both 60×60 (×) and 120×120 (○) lattices at $T=T_R$.

The finite-size effect is also prominent for the 60×60 lattice at $T=T_R$, as shown in Fig. 2. My MC simulation was considerably shorter than that of SWG (4×10^4 MCS/S vs 1.22×10^6 MCS/S for SWG), but nevertheless provided sufficient accuracy to see the major effects.

The decrease of $B(r)$ as r increases is about the same as for $T=2T_R$. Its identity as being largely a finite-size effect is confirmed by comparison with MC data for a 120×120 system (2.16×10^4 MCS/S), also shown in Fig. 2.

However, the data for $B(r)$ at $T=T_R$ lies considerably *above* the exact asymptotic value in the region considered by SWG. Averaging over all data for $7\leq r\leq12$, I find calculated values of B that are $10(\pm5)\%$ too high for 60×60 and $20(\pm3)\%$ too high for 120×120, using SWG's procedure.

This systematic error is also not surprising, considering that the distance between vortex pairs in the KT theory has been estimated to be about ten lattice constants.[6] Correlation functions are not expected to reach their asymptotic behavior unit $r\gg10$, as had been pointed out prior to SWG's paper.[6] [At higher temperatures, the KT pairs are much further apart, but their effect on $G(r)$ is correspondingly less.] As seen from Fig. 2, the MC data for the 120×120 lattice seem to be approaching the asymptotic value slowly from above as r increases, although they might still contain significant finite-size effects.

I also disagree with SWG that their method is superior to considering the size dependence of

$$\omega(N)=\langle(h_i-\langle h_i\rangle)^2\rangle_N\ , \tag{3}$$

where the average is taken over an $N\times N$ lattice with periodic boundary conditions. This quantity should also diverge logarithmically

$$\omega(N)\rightarrow A\ln N+\text{const} \tag{4}$$

with $A=\frac{1}{2}B$ (so that $A=2/\pi^2$ at $T=2T_R$ and $A=1/\pi^2$ at $T=T_R$).

The crosses in Fig. 3 are MC data for $\omega(N)$ vs $\ln N$ for $T=2T_R$. The straight line is a fit through the points for $N=7$, 10, 14, and 20, and yields a value for A that is $1.3(\pm2.0)\%$ above the asymptotic value. The error is probably entirely statistical, since the systematic error for the corresponding Gaussian model is less than 0.1% in this range.[6] Using the SWG method, I had a *statistical* error of only 1.5%, but this required seven times as much computer time as the total for all six lattice sizes used for $\omega(N)$ in Fig. 3. Consequently, per unit of computer time, using $\omega(N)$ produces smaller statistical errors than using SWG's $G(r)$, as well as effectively eliminating the systematic error for $T=2T_R$.

Figure 3 also contains MC data at $T=T_R$. The ap-

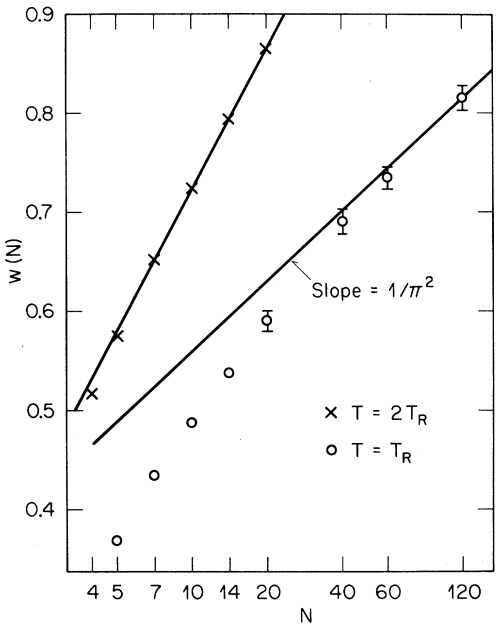

FIG. 3. MC data for $\omega(N)$ vs $\ln N$ for the BCSOS model at $T=T_R$ and $T=2TR$.

proach to the asymptotic behavior is much slower[6] and even the points for $N=40$, 60, and 120 are not convincingly in the asymptotic region. These methods do not accurately determine the asymptotic behavior at the transition.[15]

Of course, we can also use $\omega(N)$ to estimate T_R *(assuming* the validity of the KT theory). Estimates of transition temperatures for the solid-on-solid (SOS) and discrete Gaussian (DG) models can be read directly from Fig. 7 of Ref. 7 and Fig. 9 of Ref. 6. This gives $T_R(\mathrm{SOS})=1.21\pm0.01$ and $T_R(\mathrm{DG})=1.44\pm0.02$ (the errors refer only to MC statistics), roughly the same as SWG. This would also mean that the MC data in Refs. 6 and 7 are consistent with the KT theory prediction[5,8,16,17] that the step specific heat goes to zero at T_R with an essential singularity.

Although the SWG method of fitting B in Eq. (1) to the KT theory is useful for finding the transition temperature, it is not superior to fitting A in Eq. (4) for this purpose, and it does not test the validity of the KT theory. As SWG were aware, even if the comparison with the BCSOS model had not shown deviations from the expected asymptotic behavior, this approach still would not have tested the KT theory for other models since we do not, in general, have an independent determination of the transition temperature.

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