Properties of the q-state clock model for $q=4$, 5, and 6

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The two-dimensional clock models for $q=4$, 5, and 6 were simulated on lattices of size 256 and 1024. Various properties were computed including the specific heat, susceptibility, vorticity, and correlation times. However, only a Monte Carlo renormalization-group analysis was capable of locating quantitatively the phase transitions for $q=5$ and 6. The results agree with the qualitative picture obtained for the Villain version of the clock model. The relevance of this work to the two-dimensional melting problem is discussed.
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I. INTRODUCTION

Recently a series of computer simulations of melting in two dimensions (2D) has generated a great deal of controversy over the nature of the phase transformation from solid to liquid.[1,2] The data from these computer experiments are interpreted as either the result of a first-order transition as in three dimensions or as the result of a sequence of two second-order transitions of the Kosterlitz-Thouless (KT) type.[3] In addition to searching for the solution to this particular problem, the computer simulations have spurred the development of more careful and sophisticated analyses.

To determine what the best method of analysis would be, I have simulated the q-state clock model which, for q sufficiently large, has three phases analogous to those postulated by Halperin and Nelso (HN) for 2D melting.[4] The clock models are 2D planar spins where the spins are restricted to q evenly-spaced orientations. At low temperatures there is an Ising-type ordered phase with long-range correlations. For q large enough (thought to be $q>4$) there is an intermediate phase similar to the low-temperature phase of the 2D planar model where spin-spin correlations fall off as $1/r^{\eta}$, where η is a temperature-dependent critical exponent.[5-7] At high temperatures there is a disordered phase with exponentially decaying correlations.

The analogous situation for the HN theory of 2D melting is the following. There is a low-temperature phase of long-range correlations between the orientation of the bonds connecting nearest-neighbor particles. However, the positional correlations [i.e., the peak heights in the pair-distribution function $g(\vec{R})$] decay as a power law indicating the lack of long-range positional order. This phase is destroyed by the dissociation of dislocation pairs to form an hexatic phase with orientational correlations falling off as a power law and positional correlations falling off exponentially. The hexatic phase is then destroyed by the dissociation of disclination pairs and a liquid phase, with exponentially decaying correlations, is created. The difficulty in the simulations is locating an hexatic phase and distinguishing it from the possibility of two-phase coexistence between liquid and solid. In all simulations done so far, large correlation times have been observed at intermediate temperatures making it difficult or impossible to reach thermodynamic equilibrium (or at least to use enough states to compute averages reliably).

The purpose of this work is first to obtain accurate data for the clock models considered, second, to see if effects found in 2D melting are found here and, third, to determine what are the best methods of analysis to understand the physics of these systems. Also, since this system is expected to behave like the analogous four-dimensional gauge theories, the results here may be of some value to particle theorists.

In the next section I present the model and the computational procedure. In Sec. III the results for various quantities are presented. In particular I will be using the Monte Carlo renormalization group (MCRG) as a powerful tool of analysis.[8] Finally, in Sec. IV a discussion of the relevance of the results to the 2D melting problem is given.

II. COMPUTATIONAL PROCEDURE

The reduced Hamiltonian for the q-state clock model (also called the vector Potts model) is

$$H=\frac{-1}{T}\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)\ ,$$

$$\theta_i=\frac{2\pi p}{q},\ p=1,2,\ldots,q\ , \quad (1)$$

where the sum is over nearest-neighbor pairs on a square lattice with periodic boundary conditions.

The algorithm for updating spins was the usual Metropolis rule. A trial move consisted of randomly turning a spin one unit to the left or one unit to the right. Turning more than one unit would be an unlikely event except at high temperatures; thus we discard this possibility. The spins to be updated were chosen sequentially in the order in which they are labeled. Thus, one less random number per update is needed and it allows spin-wave-type excitations to occur more easily. One expects this procedure to improve the sampling of phase space. Using this procedure the time to update one spin was about 90 μsec on the 190L array processor of Floating Point Systems, Inc. using a compiled program.

For the 256 spin system 30 000 passes through the lattice were averaged over and 6000 passes were skipped for the purpose of equilibration. For 1024 spins, 50 000 passes were averaged over and 10 000 to 20 000 passes were skipped. Averages were computed every five passes and standard deviations were computed by dividing the averages into ten data points. All errors quoted in this paper are based on one standard deviation error bars, even though there may be larger systematic errors which are difficult to determine. Runs were begun either by heating or cooling from the last configuration of a previous run, usually 0.1 away in temperature. Correlation times of most quantities were computed to ensure that the running time was sufficient. The program was tested by comparing the computed energy with that of the low-temperature expansion (see Appendix) and with exact results for $q=4$.[9]

III. RESULTS

A. Energy

Table I shows the energy for the clock models as a function of temperature in heating runs of 256 spin lattices. For $q=5$ a cooling run was also done and the energy data were found to be approximately within 1.0% of the heating run. The energy for 1024 spins is slightly higher ($\sim$1.0% higher) reflecting the fact that the periodic boundary conditions cause the smaller system to be more correlated.

Figure 1 shows the specific heat C for all three values of q. These data are equal to $\Delta E/\Delta T$ with $\Delta T=0.1$ in most cases. As can be seen there are

TABLE I. Energy as a function of T and q for $N=256$ and heating. Error estimates are one standard deviation error bars.

T	$q=4$	$q=4$ (exact) Infinite lattice	$q=5$	$q=6$
0.3				-1.9941 ± 0.0002
0.4				-1.9663 ± 0.0002
0.5			-1.9730 ± 0.0002	-1.8932 ± 0.0007
0.6			-1.9250 ± 0.0005	-1.7616 ± 0.0015
0.7			-1.8367 ± 0.0007	-1.6433 ± 0.0011
0.8	-1.9269 ± 0.0004	-1.9263	-1.6911 ± 0.0017	-1.5495 ± 0.0007
0.9	-1.8579 ± 0.0010	-1.8591	-1.5474 ± 0.0018	-1.4535 ± 0.0012
1.0	-1.7419 ± 0.0024	-1.7456	-1.4034 ± 0.0021	-1.3406 ± 0.0025
1.1	-1.5500 ± 0.0038	-1.5463	-1.2757 ± 0.0016	-1.1957 ± 0.0030
1.2	-1.2708 ± 0.0053	-1.2266	-1.1157 ± 0.0026	-1.0598 ± 0.0027
1.3	-1.0356 ± 0.0027	-1.0280	-0.9929 ± 0.0018	-0.9438 ± 0.0012
1.4	-0.9057 ± 0.0016	-0.9096	-0.9101 ± 0.0017	-0.8533 ± 0.0015
1.5	-0.8177 ± 0.009	-0.8172	-0.8341 ± 0.0008	-0.7785 ± 0.0013
1.6			-0.7644 ± 0.0016	-0.7191 ± 0.0011
1.7			-0.7141 ± 0.0016	-0.6671 ± 0.0016
1.8			-0.6710 ± 0.0012	-0.6249 ± 0.0013
1.9			-0.6277 ± 0.0014	-0.5850 ± 0.0009
2.0				-0.5509 ± 0.0010
2.1				-0.5166 ± 0.0011
2.2				-0.4914 ± 0.0011

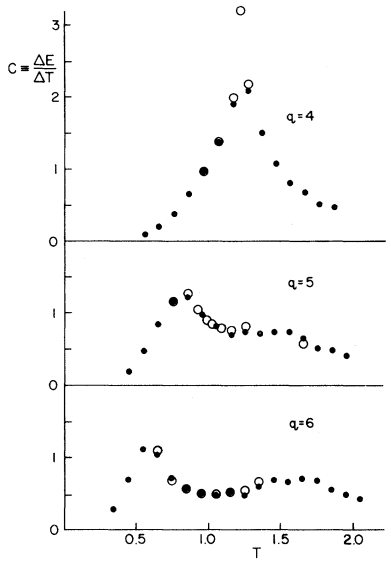

FIG. 1. Specific heat as a function of temperature. ○ designates 1024 spins; ● designates 256 spins.

two peaks in C for $q=5,6$ and only one for $q=4$. This suggests there are two phase transitions for $q \geq 5$. As we shall see in a moment these two peaks are not located near the phase transitions. For $q=4$ the single peak is located near T_C and there appears to be some size dependence to the height of the peak as one expects for the standard second-order phase transition.

B. MCRG

The most reliable method for determining the location of critical points is MCRG.[8] The method involves matching thermodynamic averages of block spins on lattices of the same size which originated from two lattices, one of size 1024 spins and the other 256 spins. If T_1 and T_2 are the temperatures of the two original spin lattices at matching, then $\Delta T \equiv T_2 - T_1$ is a discrete version of the beta function, and tells one how the temperature is renormalized by a scale change of $b=2$. If $\Delta T=0$ we have a critical point. $\Delta T<1$ is an ordered phase and $\Delta T>0$ is a disordered phase.

The blocking rule is defined by vectorally summing four spins on a plaquette and choosing the block spin to be that vector closest in direction to the sum. The block spins also have q possible states. Ties and sums adding to zero were eliminated by favoring slightly one of the four spins forming a block spin. This blocking was continued until we were left with a 2×2 lattice.

To determine ΔT quantitatively I used

$$E^{(m)}(N) \equiv \sum_{\langle ij \rangle} \cos(\theta_i^{(m)} - \theta_j^{(m)}) , \tag{2}$$

where $\theta_i^{(m)}$ is the angle of the block spin at site i after m blockings from a lattice of N spins. The vorticity of the blocked spins also matched giving the same ΔT. The quantity

$$\left\langle \left[\sum_i \cos\theta_i^{(m)} \right]^2 + \left[\sum_i \sin\theta_i^{(m)} \right]^2 \right\rangle \equiv \langle (S_T^{(m)})^2 \rangle , \tag{3}$$

was also computed, but it had larger error bars and showed hysteresis between heating and cooling. The matching was carried out by plotting $E^{(m)}$ (256) and $E^{(m+1)}$ (1024), drawing a smooth curve through the data points for $E^{(m)}$ (256) and reading off ΔT. An example is shown in Fig. 2. The error bar for this procedure is around ± 0.01 near the transitions. The data for a case where $\Delta T=0$ is shown in Table II. Generally, matching occurs on two to three length scales. (At least two scales are needed to be certain of the values.)

The results for ΔT as a function of T_1 (the temperature of the 1024 spin system) are shown in Fig. 3. For $q=6$ there are clearly three phases, an Ising-type ordered phase ($\Delta T<0$), an x-y-like phase ($\Delta T=0$), and a disordered phase ($\Delta T>0$). The boundaries of the three phase are at $T_{\mathrm{I}} \approx 0.6$ and $T_{\mathrm{II}} \approx 1.3$. For $q=5$ the x-y-like phase is much narrower, as expected, with $T_{\mathrm{I}} \approx 0.8$ and $T_{\mathrm{II}} \approx 1.1$. These estimates are probably accurate to within 10% and are reliable since they are the same with heating and cooling, tested for the $q=5$ systems. For $q=4$ there is only one phase transition and we

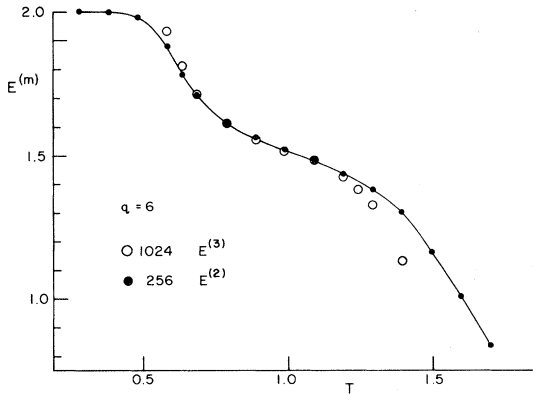

FIG. 2. Examples of $E^{(m)}$ vs T used to compute ΔT. Error bars are smaller than the symbol size.

TABLE II. Matching of $E^{(m)}(N)$ for $q=6$, $T=1.0$.

Block lattice	Original lattice $N=1024$	$N=256$
32×32	1.3317 ± 0.0019	
16×16	1.3775 ± 0.0026	1.3406 ± 0.0025
8×8	1.4170 ± 0.0058	1.3770 ± 0.0051
4×4	1.4485 ± 0.0077	1.4326 ± 0.0069
2×2	1.6134 ± 0.0093	1.6062 ± 0.0102

find $T_c=1.11\pm0.03$, compared to the exact result $T_c=1.1346\ldots$.[9]

With the use of the fact that the correlation lengths at T_1 and T_2 differ by a factor of 2, we can obtain the critical exponent ν, which characterizes the divergence of the correlation length, by the formula

$$\nu=\ln 2/\ln\left[1+\frac{d\Delta T}{dT_{\mathrm{I}}}\right]. \tag{4}$$

For $q=5$ and 6, $\nu=\infty$ if ΔT is a differentiable function of T as we expect. (It might not be for a first-order transition.) This is consistent with the prediction that T_{I} and T_{II} are Kosterlitz-Thouless transitions.[5–7] For $q=4$ we find $\nu=1.25\pm0.20$. $\nu=1$ is the exact result since the four-state clock model is equivalent to two decoupled Ising models.[9]

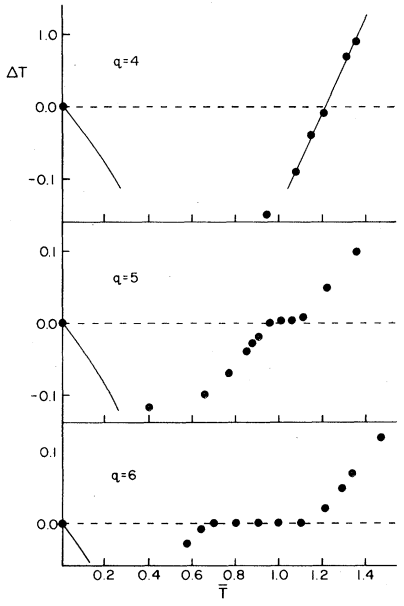

FIG. 3. ΔT vs T_1 (1024 spin temp.). The low-temperature curves are the result of a low-temperature renormalization group. Error bars are approximately ±0.01 for data near $\Delta T=0$.

For comparison $\nu=1.07\pm0.15$ for the Ising model in two dimensions using one million passes on a 256-spin lattice matched to a 64-spin lattice.[10]

C. Spin rescaling

The critical exponent η can be determined by noting that when $\Delta T=0$ we have

$$\langle (S_T^{(m)})^2\rangle \sim (N^{(m)})^{1-\eta/d}, \tag{5}$$

where $N^{(m)}$ is the size of the mth block lattice and $d=2$ is the dimension of the lattice. In general the data for the above quantity exhibits very large fluctuations similar to those explained below in Sec. III D; however, the data where the value for η is not unreliable to much more than 20% is shown in Table III. In general for $\Delta T\neq0$ a log-log plot of the data shows a curve instead of a straight line indicating correctly that it is not critical.

Analysis on the Villain model predicts that η varies in the intermediate phase from $4/q^2$ to $1/4$.[5–7] Our data are consistent with this prediction at least near T_{I}.

For $q=4$ we find $\eta=0.18$ at $T=1.1$ and $\eta=0.33$ at $T=1.2$. (We used the best straight-line fit even if there is a little curvature.)

D. Order parameter

The magnetization and susceptibility are defined as

$$\langle\vec{\mathrm{M}}\rangle\equiv\left\langle\sum_i\cos\theta_i,\sum_i\sin\theta_i\right\rangle, \tag{6}$$

$$\chi\equiv 1/N(\langle M^2\rangle-\langle M\rangle^2). \tag{7}$$

$\langle\vec{\mathrm{M}}\rangle$ drops sharply in magnitude at T_{I} and then stays roughly constant at a value 15–20% of per-

TABLE III. η as a function of T. $T/2\pi$ is the lowest-order spin-wave prediction. These data are accurate to around 10–20%.

T	$T/2\pi$	η $q=5$	$q=6$
0.6	0.095		0.10
0.7	0.111	0.07	0.15
0.8	0.127	0.16	0.19
0.9	0.143	0.17	0.24
1.0	0.159	0.28	0.32

fect alignment at least up to $T=2.0$ $\langle M^2\rangle/N$ exhibits huge fluctuations in the x-y-like phase as shown in Fig. 4. Apparent hysteresis due to these fluctuations occurs for $N=256$ where for $q=5$, $T=0.8$, $\langle M^2\rangle/N=210$ (heating) and 100 (cooling). The susceptibility rises sharply near T_{I}, remains large in the x-y-like phase and slowly decreases as the temperature increases in the disordered phase. Because all of these quantities are very sensitive to long-range fluctuations, it is not surprising that their statistical fluctuations are large. If these were the only quantities we measured we would have a very confusing picture of the phase structure of this system.

E. Vortices

Einhorn *et al.*[6] give a description of the phase transitions in the clock models in terms of topological defects. The transition between the ordered phase and the x-y-like phase is described as a condensation of droplets of spins rotated with respect to the net magnetization. The boundary of a droplet is a closed string in analogy to the language used in particle physics. Vortices, defined as a topological defect where the change in θ around a closed loop is nonzero, are tightly bound by a linear potential (not logarithmic as in the x-y model because θ_i is discrete). A vortex pair is a positive and negative vortex connected by strings. In the x-y-like phase the potential between vortices is reduced on larger length scales to a logarithmic potential (i.e., imagine averaging groups of spins so that the change in the averaged spin as a function of position becomes more and more continuous. Note, this is not a blocking transformation which maintains the symmetry of the spin). The transition from an x-y-like phase to a disordered phase is then just that of a Kosterlitz-Thouless vortex pair unbinding mechanism.

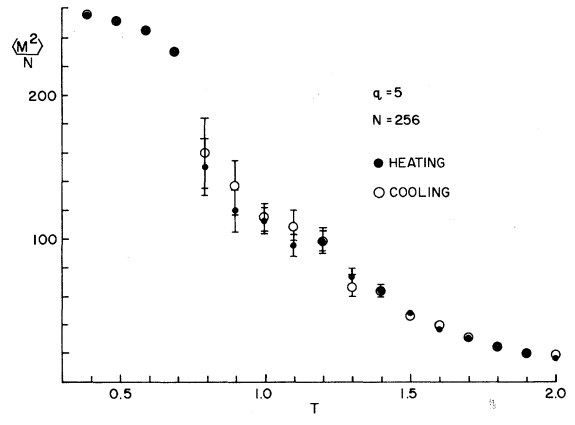

FIG. 4. $\langle M^2\rangle/N$ as a function of T, heating and cooling.

In this simulation the vorticity is computed for each plaquette. If v is the number of vortex pairs per spin then a plot of $\ln v$ versus $1/T$ gives a straight line at low temperatures (Arrhenius law). From this the chemical potential to create a pair of vortices is found to be $2\mu=7.3$ for $q=6$, 8.2 for $q=5$, and 10.6 for $q=4$. The value found for the planar model was $2\mu=10.2$[11] At high temperatures v deviates from the Arrhenius law. This occurs at $T\approx 1.3$ for all q. At $T=1.2$, $v=0.025$ for $q=4$ and 5, and $v=0.035$ for $q=6$.

Plots of the location of the vortices were also generated. The results showed that generally at temperatures below T_{II} there were no vortex pairs where the separation between members of the pair were more than three lattice spacings. Above T_{II} there usually appeared some vortices that appeared to be unbound, although this is somewhat of a subjective result. The lifetime of many vortex pairs is only around one pass, suggesting that they are not true excitations. Also, note that near T_{II} in the 1024-spin lattice there are only about 30 vortex pairs. These vortices are clearly not able to perform the screening that is used in the KT theory to derive quantitative results. Nevertheless the MCRG results seem quite plausible. Just as MCRG is expected to give reliable information on the infinite lattice even though the lattices simulated are much smaller than the correlation length, it appears here to also work even though the mechanism which drives the transition appears to operate on a scale larger than the lattices used.

Finally, we note that in this system there appeared to be much less clumping than was found in the planar model or the two-dimensional melting models that have been simulated.[1,2,11]

F. Dynamics

The time-correlation function for $E^{(m)}$ and $\langle (S_T^{(m)})^2\rangle$ were computed. In all cases the correlation times for these quantities were much smaller than the duration used for each data point, thus insuring that the computation of error bars is reliable. This does not prevent systematic errors due to extremely long correlation times which are not detected by the above computation. This can be tested to

some degree by heating and cooling the systems as we have done for $q=5$.

The behavior of the correlation time τ for $\langle M^2 \rangle$ for $N=256$, as a function of temperature was as follows: For very low temperatures τ is essentially zero; each pass is independent of the next. The dynamics is such that isolated spins are turning occasionally, and then returning to their original orientation. τ then begins to rise to around ten passes just below $T_{\rm I}$ and then rises sharply to around 500 passes at $T_{\rm I}$. In the x-y-like phase τ decreases from 500 to around 50 passes. As the temperature is increased beyond $T_{\rm II}$, τ decreases gradually to around ten passes at $T=1.8$ for $q=5$ and 6. The correlation time for the energy is difficult to determine because it does not fluctuate very much and computing $\langle E(t)E(0)\rangle - \langle E\rangle^2$ is very small, comparable to the computer precision.

For $E^{(m)}$, $m>1$ we can compute the correlation time $\tau^{(m)}(N)$. With the use of these quantities as a measure of the time scales for the blocked lattices, we can employ dynamic MCRG (Ref. 10) to obtain the dynamic critical exponent z whenever $\Delta T=0$. This is given by the formula

$$\frac{\tau^{(m+1)}(1024)}{\tau^{(m)}(256)} = b^z = 2^z \,. \tag{8}$$

With the use of this formula z is typically between 1.3 and 1.8 in the x-y-like phase for $q=5$ and 6. The error bars on $E^{(m)}$ are generally large. At $T=1.2$, $z\approx 1.6$ for $q=4$.

z was also computed by matching the block spin-autocorrelation functions $\langle \cos[\theta_i^{(m)}(t)-\theta_i^{(m)}(0)]\rangle$. In this case t plays the role of τ in Eq. (8). The results were obtained for $q=6$, and showed that $z\approx 1.6$ consistent with those above.

The above values are considerably lower than those found for the 2D Ising[10] and three-state Potts models,[12] where $z=2.2$ and 2.7, respectively. Also, z is not a monotonic function of q for small q.

IV. DISCUSSION

The results in Sec. III tell us a great deal about what quantities are the most useful for understanding the phase transitions of clock models and other similar systems. The specific heat tells us there are likely to be two transitions for $q=5$ and 6, but does not tell us where the transitions are located. The magnetization and susceptibility also give inaccurate estimates of the transitions as well as having large error bars and hysteresis. Knowledge of the number and location of the vortices again is inconclusive. The dynamics, although interesting and suggestive, are not very precise. Only MCRG gives a clear and quantitative picture of the phase transition.

If we now consider the 2D melting problem where the lattices are of comparable size and running times somewhat less, we might expect the same kind of results. In fact, the situation is probably more complicated since there is not a fixed lattice and the potentials used are generally more complicated than those used here. Only thermodynamic quantities, correlation functions, and pictorial displays of defect and particle configurations have been computed for 2D melting systems, which in the present work are found to be inaccurate and sometimes misleading.

If one compares the results of 2D melting simulations with those of the present work, one finds qualitative similaritiies. Large, long-lived fluctuations and hysteresis exist in long-range quantities (the energy in most melting problems is also somewhat long-range, extending over a few to infinite numbers of particle spacings). Correlation functions exhibit large fluctuations and long correlation times throughout the controversial temperature range.[1,2,13] The only aspect which appears somewhat different is that the clock models appear to have fewer defects and less clumping than in melting or in the planar model. This probably accounts for the broader specific heat peaks found here compared to the planar model.[11] However, we must emphasize that no simulation has been run longer than the characteristic times for defect motion.

In conclusion, we have obtained quantitative information on the clock models for $q=4$, 5, and 6 using MCRG which agrees with the picture obtained by analyzing the Villain version. Our results suggest that simulations of 2D melting should focus on short-range quantities such as near-neighbor translational and orientational correlations and that a MCRG procedure should be devised. This approach is currently in progress.

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APPENDIX: LOW-TEMPERATURE EXPANSION

The low-temperature expansion for $E^{(0)}$ for the q-state clock model is[14]

$$E^{(0)}=2-\Delta\epsilon(8u^4+24u^6+\cdots),$$

where

$$\Delta\epsilon=1-\cos(2\pi/q) \tag{A1}$$

and

$$u=\exp(-\Delta\epsilon/T).$$

The first term in parentheses is due to a single spin turning one unit from perfect alignment and the second term is that due to two neighboring spins turning one unit in the same direction. Using our block rule, one finds

$$E^{(1)}=2-\Delta\epsilon(3u^6+\cdots). \tag{A2}$$

The single-spin excitations have no effect on blocking and the double-spin excitations remain only half the time if the two spins are in the same plaquette which occurs only one fourth the time. Matching occurs when $E^{(0)}(T)$ and $E^{(1)}(T-\Delta T)$ are equal. To first order this gives

$$\Delta T=T\left[1-\frac{1.5}{1-AT}\right] \tag{A3}$$

where $A=\ln(\frac{8}{3})/4\Delta\epsilon$. This simple renormalization group gives $\Delta T<0$ for q finite and $\Delta T=0$ for $q\to\infty$ as desired.

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