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Finite-size effects on the critical structure factor of the two-dimensional Ising model

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Abstract. Explicit calculations of the critical structure factor of the planar Ising model on square lattices with a variety of boundaries are compared with the results of conformal invariance. Monte Carlo is used for square, circular and 2×1 rectangular geometries with free boundary conditions; transfer matrices are used for an infinite strip with periodic boundary conditions. Good agreement is found for wavevectors less than a quarter of a reciprocal lattice spacing. An appendix shows how symmetries can be used to simplify computing, from transfer matrices, the structure factor in the 'infinite direction'.

Critical correlation functions are believed to be invariant under conformal transformations. There is thus a relationship between the correlation functions of systems which have different geometries but which can be mapped into each other with a conformal transformation. Using the known two-point correlation function for the two-dimensional Ising model on a semi-infinite plane, Kleban *et al* (1986) (hereafter referred to as KAHB) have used conformal invariance to compute the correlation functions of Ising models in circular and rectangular regions with free boundaries. Cardy (1984) has computed the pair correlation function for systems defined on infinite cylinders given the critical correlations on an infinite plane for operators with any anomalous dimension (Hentschke *et al* 1986). The purpose of this work is to present numerical evidence, in the form of Monte Carlo and transfer matrix calculations, which can be compared with these results. While this manuscript was being prepared, we learned of similar Monte Carlo work by Badke *et al* (1985) for the case of the circular geometry. However, we average over at least two orders of magnitude more lattices and also we compare structure factors (the Fourier transforms of the correlation functions) rather than the correlation functions themselves. We find that the structure factors obtained by conformal invariance accurately ($\pm 3\%$) represent the structure factors of systems of only a few thousand sites as long as the wavevector is less than $\pi/2a$ (with a the lattice spacing).

The structure factor of the Ising model is defined as

$$S(\boldsymbol{k}, T) = \left\langle \left| \sum_i \sigma_i \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i) \right|^2 \right\rangle \tag{1}$$

where $\sigma_i = \pm 1$ is the value of the spin on site i. Finite-size scaling theory applied to the structure factor yields the hypothesis that in the scaling limit, $L\to\infty$, $\xi\to\infty$, and

$k \to 0$ but with $k\xi$ and kL fixed,

$$S(k, T, L) \sim L^{4-\eta} X_{\pm}(k\xi, kL). \tag{2}$$

The calculations of KAHB yield the critical correlations, i.e. the limit $k\xi \to \infty$, for which finite-size (and hence boundary and geometrical) effects are important even in the infinite system limit

$$S(k, T_c, L) \sim \lim_{x \to \infty} L^{4-\eta} X_{\pm}(x, kL) = L^{4-\eta} Y(kL) \equiv S^*(k). \tag{3}$$

The strategy of what follows is first to show how accurately the critical correlations obtained in the numerical studies satisfy the scaling form of (3) for various k and L, and then to determine how accurately the explicit scaling functions $Y(y)$ determined by KAHB represent the data.

First, using Monte Carlo, the structure factor of the two-dimensional Ising model on a square lattice was computed for three different geometries with free boundary conditions: (1) square, (2) circular and (3) 2×1 rectangular. The structure factor, defined by (1) and scaled according to (3), for the square case is shown in figure 1. The wavevectors are parallel to one of the edges of the lattice. The number of Monte Carlo steps per site performed to compute $S^*(k)$ varied from 5×10^6 for the smaller lattices to 2×10^5 for the largest. By observing the size and 'time' scale of the fluctuations we estimate the structure factors at small k for the larger lattices to be accurate to within at least 3%. The structure factor was computed every 10 to 50 Monte Carlo steps (again depending on the lattice size) after the first ~10% of the steps were discarded to allow for equilibration from the initial (usually ordered) configuration.

Our first observation is that the computed structure factors satisfy the scaling form of (3) within the accuracy of the Monte Carlo data when $k \leq \pi/2a$ (figure 1). The

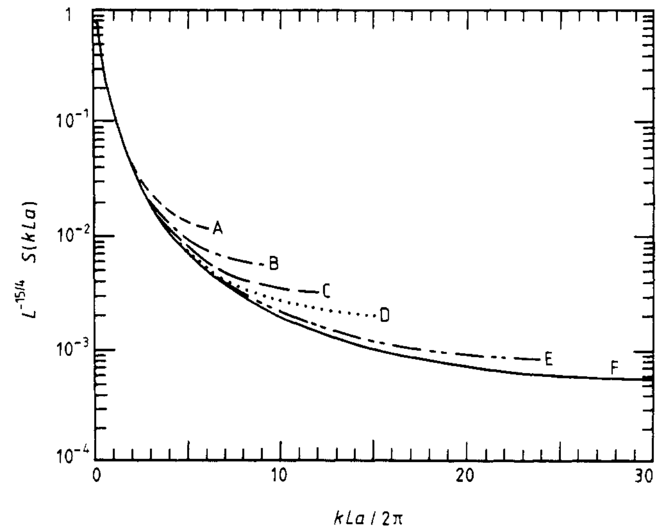

Figure 1. Scaled critical structure factors obtained from Monte Carlo calculations for the Ising model on a square lattice of square geometry ($L \times L$) with free boundary conditions; k is along a principal axis. A, $L = 12$; B, $L = 18$; C, $L = 24$; D, $L = 30$; E, $L = 48$; F, $L = 60$.

validity of finite-size scaling for rather small L has, of course, been observed before (Barber 1984). The breakdown of scaling for the Ising model only at length scales comparable to the lattice spacing is expected (Aharony and Fisher 1980). Figures 2 and 3 show similar results for circular and rectangular regions respectively. In figure 2, L is the number of lattice sites along a diameter of the circle. The rectangular region of figure 3 has a width half of its length; L is the number of lattice sites in the direction of the short dimension. Figures 3(a) and 3(b) contain scaled structure factors for wavevectors in the short (k_x) and long (k_y) direction, respectively.

To compare these structure factors with the results of KAHB we need to determine a normalisation factor. The critical spin-spin correlation function of the Ising model decays at large r as (McCoy and Wu 1973)

$$\langle \sigma_0 \sigma_r \rangle \sim \frac{2^{1/8} A}{(r/a)^{1/4}}, \tag{4}$$

where the constant A is 0.645 022 .... The structure factor of KAHB is defined by

$$S^*_{\mathrm{CI}}(\boldsymbol{k}) = \int \mathrm{d}^2 r_1 \int \mathrm{d}^2 r_2 \, g(\boldsymbol{r}_1, \boldsymbol{r}_2) \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}), \tag{5}$$

where the correlation function $g(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is normalised so that it approaches $|\boldsymbol{r}_1 - \boldsymbol{r}_2|^{-1/4}$ as $\boldsymbol{r}_1$ approaches $\boldsymbol{r}_2$. When $|\boldsymbol{k}| \ll \pi/a$ and a is much less than the system size, the integrals in (5) can be replaced by summations and $g(\boldsymbol{r}_1, \boldsymbol{r}_2)$ by $\langle \sigma_{r_1} \sigma_{r_2} \rangle / (2^{1/8} A a^{1/4})$. Thus, in this limit, $S^*_{\mathrm{CI}}(\boldsymbol{k})$ is proportional to the $S^*(\boldsymbol{k})$ defined by (3):

$$S^*_{\mathrm{CI}}(\boldsymbol{k}) \approx a^2 \sum_{r_1} a^2 \sum_{r_2} \frac{\langle \sigma_{r_1} \sigma_{r_2} \rangle}{2^{1/8} A a^{1/4}} \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2)] = \frac{a^{15/4}}{2^{1/8} A} S^*(\boldsymbol{k}). \tag{6}$$

For a square boundary defined to have an edge length of 2 (as in KAHB), $a = 2/L$

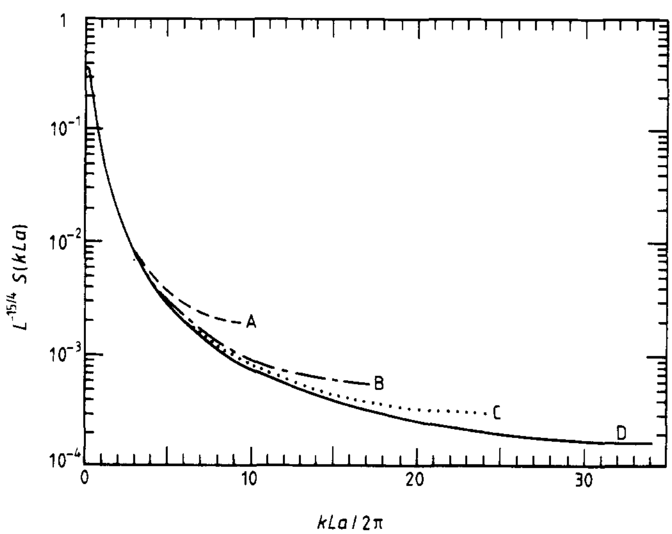

Figure 2. Scaled critical structure factors for circular geometry (diameter L) with free boundary conditions. A, $L = 19$; B, $L = 35$; C, $L = 49$; D, $L = 69$.

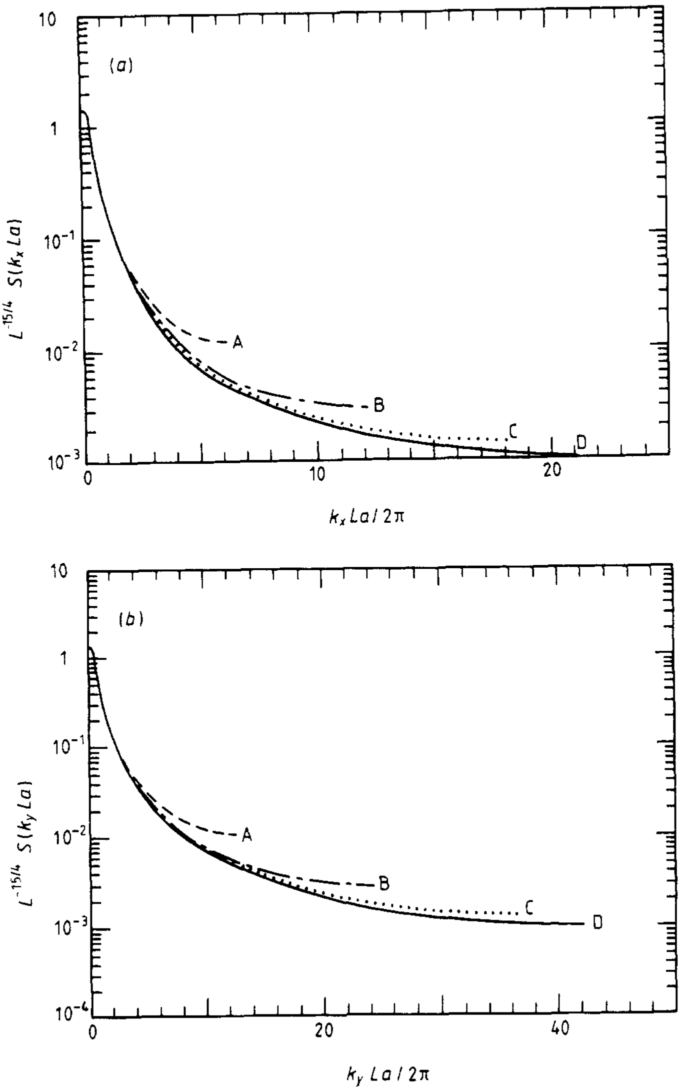

Figure 3. Scaled critical structure factors for a rectangle with the width half the length ($L\times 2L$) and with free boundary conditions; (A, $L=12$; B, $L=24$; C, $L=36$; D, $L=42$). (*a*) along the shorter direction, (*b*) along the longer direction.

where L is the number of sites along a boundary, and so

$$L^{-15/4}S^*(0)=2^{-29/8}AS^*_{\mathrm{CI}}(0). \tag{7}$$

This equation is also valid for the unit circle when L is the number of sites along a diameter, and for a 2×4 rectangle when L is the number of sites along the shorter dimension. Table 1 compares our Monte Carlo results with the predictions of conformal invariance.

The effective amplitudes of the $L^{15/4}$ divergence of $S^*(0)$ decrease with increasing L. It is difficult to extrapolate to the largest L limit because for the largest lattices considered the uncertainty in $S^*(0)$ is comparable to finite-size effects. Given this uncertainty, and the uncertainty in the Monte Carlo data and in the conformal

Table 1. Values of $L^{-15/4}S(0)$ obtained by Monte Carlo calculation compared with the predictions of conformal invariance for three different geometries.

	2×2 square		Unit circle		2×4 rectangle	
	L	$L^{-15/4}S(0)$	L	$L^{-15/4}S(0)$	L	$L^{-15/4}S(0)$
Monte Carlo	12	0.420	19	0.277	12	1.32
	18	0.406	35	0.259	24	1.26
	24	0.388	49	0.256	36	1.27
	30	0.386	69	0.251 ± 0.007	42	1.21 ± 0.04
	48	0.378				
	60	0.374 ± 0.010				
Conformal invariance		0.346 ± 0.013		0.2482		1.08 ± 0.05

invariance results for the square and rectangular lattices (which comes from approximating a multi-dimensional integral by a sum over a finite mesh), $S^*(0)$ and $S^*_{\rm CI}(0)$ are in agreement. Notice that $L^{-2}S^*(0)$ is just the magnetic susceptibility per unit area, $\beta^{-1}\chi$, so here conformal invariance predicts the amplitude of the divergence of χ with $L^{7/4}$ just as it has (correctly) predicted the amplitude of the divergence of the correlation length with L.

Figure 4 shows $S^*(k)$ from the Monte Carlo data along a principal direction for the system with a circular boundary having a diameter of 69 sites compared with the conformal invariance results. The agreement is well within the statistical uncertainty of the Monte Carlo results. Evidently conformal invariance correctly predicts the scaling function $Y(y)$ of (3). Results for the square and rectangular geometries are also in agreement with the conformal invariance results. For example we observe the

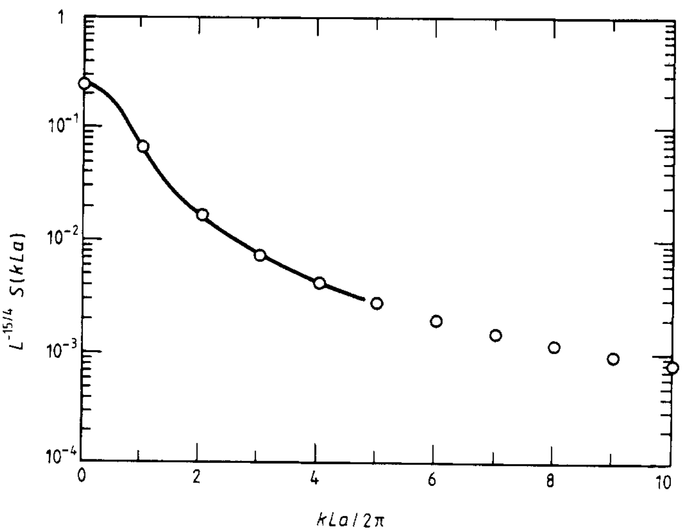

Figure 4. Prediction of conformal invariance (line) for the critical structure factor of the square Ising model on a circle with free boundary conditions compared with Monte Carlo simulations on a square lattice bounded by a circle with a diameter of 69 sites (open circles).

same effective η obtained from plots of $\log(S^*)$ against $\log(k)$ for finite k reported by KAHB, namely 0·09 for $6 \leqslant kLa \leqslant 15$ for the unit circle.

Using the conformal invariance of critical correlation functions, Cardy (1984) has computed the scaling form of the two-point correlation functions in an infinite strip of finite width with periodic boundary conditions. Using this result Hentschke *et al* (1986) have computed the critical structure factors. Using transfer matrix methods we have computed the structure factor of the Ising model for infinite strips, of width L sites, with periodic boundary conditions. Droz and Malaspinas (1983) have computed the structure factor in the infinite direction by taking second derivatives with respect to appropriate fields. Their method, however, requires a new transfer matrix for each k, and computing the matrices becomes impractical at small or nearly incommensurate k. Here, instead, we compute explicitly matrix elements needed for the row-row correlation function; we then find the Fourier transform by summing geometric series for each eigenstate and weighting the result by the matrix elements. At first glance this process would seem to require the calculation of all the eigenvalues and eigenvectors of the transfer matrix. However, as we shall show in the appendix, all that is required are the eigenvectors (and associated eigenvalues) which are invariant under cyclic permutations (and under reflection, when appropriate) of the sites of a row of a lattice. (Even further reduction is possible when, as here, there is spin inversion symmetry.) This property considerably simplifies the problem of calculating $S(k, T)$ in the infinite direction. (In the finite direction, one only needs the eigenvector associated with the largest eigenvalue (Schultz *et al* 1964), applied recently by Pesch and Kroemer (1985).)

Figure 5 shows the calculated structure factors for $L = 8, 9, \ldots, 12$. Again the data scale well for $k \leqslant \pi/2a$. The structure factors for semi-infinite strips must be normalised per row, reducing the divergence to $L^{2-\eta}$. The conformal invariance calculation

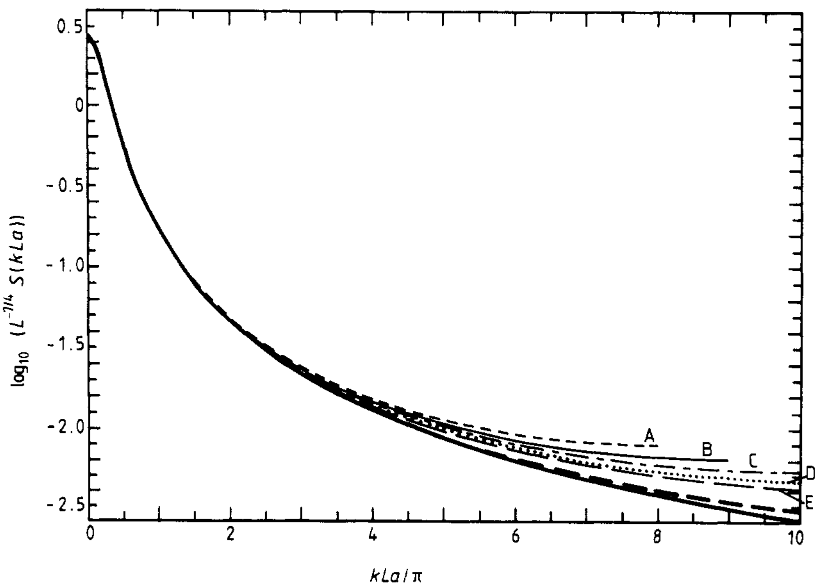

Figure 5. Prediction of conformal invariance (bold full curve) for the critical structure factor of the Ising model on an infinite cylinder compared with transfer matrix calculations for cylinder circumferences of $L = 8$ (A), 9 (B), 10 (C), 11 (D) and 12 (E) sites. The bold broken curve is an extrapolation using the data for $L = 10$, 11 and 12 (see text).

result of Hentschke *et al* (1986):

$$L^{\eta-2}S^*_{\mathrm{CI}}(k)=\frac{\pi A 2^{1/8}}{(2\pi)^{7/4}}\frac{\Gamma(7/8)}{\Gamma(1/8)}\left|\frac{\Gamma(\frac{1}{16}+\frac{1}{4}\mathrm{i}kLa/\pi)}{\Gamma(1-\frac{1}{16}-\frac{1}{4}\mathrm{i}kLa/\pi)}\right|^2 \qquad (8)$$

is also shown in figure 5, along with the estimate of the infinite L limit of $L^{\eta-2}S^*(k)$ obtained from assuming $L^{\eta-2}\tilde{S}^*(k, L)=L^{\eta-2}\tilde{S}^*(k,\infty)+bL^x$ and using $S^*(k, L)$ for $L=10$, 11 and 12 to obtain $\tilde{S}^*(k,\infty)$, b and x. Figure 6(a) plots the fractional deviation of the $L^{\eta-2}\tilde{S}^*(k,\infty)$ obtained from this extrapolation from the conformal invariance result. For kLa in the range $(0, \pi)$ and $(\pi, 5\pi)$ the fractional deviations are less than 10^{-4} and 10^{-3}, respectively, providing spectacular confirmation of the conformal invariance predictions.

Figure 6(b) shows the fitted values of x and b as a function of k. There are several noteworthy features. (1) For small k, x is near -2. (2) For large k, where scaling is expected to break down, x drops smoothly to a value near -4. (3) For $y=kLa\approx 0.27\pi$ (nearly *independent* of L) there is a singularity in the fit, with b changing sign. (Around this y, finite-size estimates of $Y(y)$ cross for all L studied.) We offer the following possible explanation of this behaviour. Since the leading corrections to scaling for the

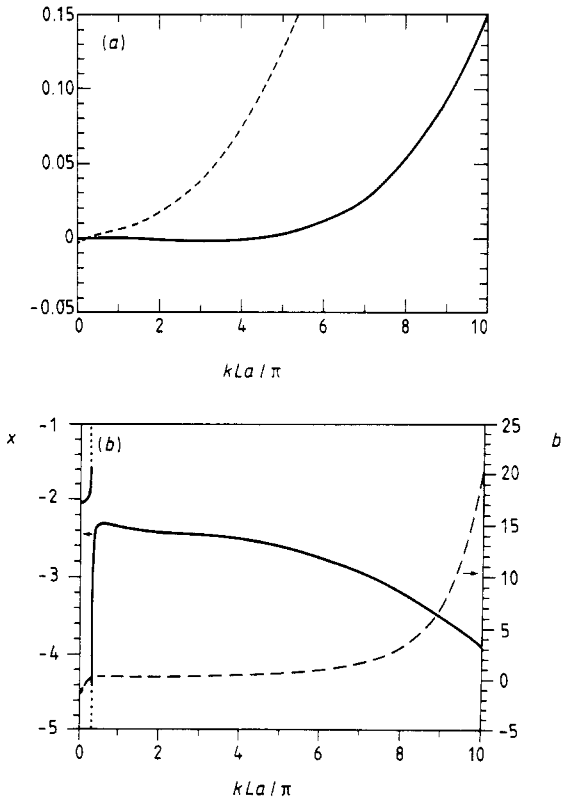

Figure 6. (a) Fractional deviation of the structure factor of the infinite cylinder from the conformal invariance predictions for finite strip with $L=11$, $\delta S^*(k, 11)$ (broken curve) $[S^*(k, 11)-S^*_{\mathrm{CI}}(k)]/S^*_{\mathrm{CI}}(k)$, and for the 10-11-12 extrapolation $\delta\tilde{S}^*(k,\infty)$ (full curve). (b) The dependence of the extrapolation exponent x (full curve) and amplitude b (broken curve) on kL for the 10-11-12 extrapolation.

2D Ising model arise from non-linearity of the scaling fields (Aharony and Fisher 1980), we replace L by $L(1+a_L L^{-2})$ and k^2 by $k^2(1+a_k k^2)$. Equation (3), normalised per spin, then becomes

$$S^*(k, L) = (L + a_L/L)^{2-\eta} Y\{[(k^2 + a_k k^4)(L + a_L/L)^2]^{1/2}\}. \tag{9}$$

This form reproduces the result (Derrida and de Seze 1982) that $(\xi^*)^2 \sim S(0)^{-1}\,\partial^2 S(0)/\partial k^2 \sim L^2(1 + a_\xi L^{-2} + \ldots)$. In the limit of small k and L^{-1},

$$S^*(k, L) \approx L^{2-\eta}[1 + (2-\eta)a_L L^{-2}][Y(kL) + \tfrac{1}{4}(a_k k^2 + a_L L^{-2})Y''(kL)],$$

so that

$$L^{\eta-2}S^*(k, L) - Y(kL) \approx L^{-2}\{(2-\eta)a_L Y(kL) + \tfrac{1}{4}[a_k(kL)^2 + a_L]Y''(kL)\}. \tag{10}$$

Thus, for small kL, we find $x = -2$, as observed. Moreover, the quantity in curly brackets vanishes at a value of kL independent of L, implying that to order L^{-2}, the left-hand side does also, consistent with the third feature. For large k, the scaling form of (9) fails to describe $S^*(k, L)$. We assume $S^*(k, L)$ is then dominated by an analytic (background) term (Privman and Fisher 1983),

$$S^*(k, L) - S^*(\pi/a, L) \propto (k - \pi/a)^2 \tag{11}$$

where $S^*(\pi/a, L) \approx 0.2978(2) + O(L^{-2})$. In the fits for figures 5 and 6, the largest y considered (the 'zone boundary') is $y_L = \pi L = y_{L+1} = y_{L+2}$. Thus $k_L = \pi/a$ but $k_{L+1(2)} \sim (\pi/a)(1 - 1(2)L^{-1})$. From equation (11), our fitting procedure at the zone boundary gives $S^* \sim L^{-2}$ (with a possible additional L^{-2} contribution from $S^*(\pi/a, L)$) or $x = -4 + \eta = -\frac{15}{4}$. At intermediate k there is smooth crossover from this limit to $x = -2$. As L increases, x becomes closer to -2 for fixed y.

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Appendix

Let T be the row to row transfer matrix for a strip of width L sites. Denote the normalised (right) eigenvector of T by $|x_s\rangle$ and the associated eigenvalues by λ_s. Then the probability that row 0, say, is in configuration i while a row r lattice spacings away in the 'positive' direction is in state j is given by (Domb 1960)

$$P_{ij}(r) = \sum_s \left(\frac{\lambda_s}{\lambda_1}\right)^r \langle e_i|x_s\rangle\langle x_s|e_j\rangle\langle e_j|x_1\rangle\langle x_1|e_i\rangle = P_{ji}(-r) \tag{A1}$$

where λ_1 is the largest eigenvalue of T and $\langle e_i|x_s\rangle$ is the ith component of the right eigenvector associated with λ_s (for generality we distinguish between the right and left eigenvectors of T, although for a square lattice this is unnecessary because the transfer matrix can be chosen as symmetric). From (1) the structure factor parallel to the infinite direction can be written as

$$S(k) = N \sum_r \langle M_0 M_r \rangle \exp(ikr) \tag{A2}$$

where M_i is the sum of spins in row i, and N is the total number of rows. In what follows we redefine S by dropping the factor of N. The correlation function $\langle M_0 M_r \rangle$ can be computed using (A1):

$$\begin{aligned}\langle M_o M_r \rangle &= \sum_i \sum_j M(i) M(j) P_{ij}(r) \\ &= \sum_s \left(\frac{\lambda_s}{\lambda_1}\right)^{|r|} \left(\sum_j M(j) \langle e_j | x_s \rangle \langle x_1 | e_j \rangle\right)\left(\sum_j M(j) \langle x_s | e_j \rangle \langle e_j | x_1 \rangle\right)\end{aligned} \tag{A3}$$

where $M(j)$ is the sum of the spins in a row with configuration j. This factorisation allows Fourier transform by summation of a geometric series:

$$\begin{aligned}S(k) = \sum_{s \neq 1} &\frac{1-(\lambda_s/\lambda_1)^2}{1 - 2(\lambda_s/\lambda_1)\cos ka + (\lambda_s/\lambda_1)^2} \langle x_1 | M | x_s \rangle \langle x_s | M | x_1 \rangle \\ &+ 2\pi\delta(k) \langle x_1 | M | x_1 \rangle^2.\end{aligned} \tag{A4}$$

We next show how symmetry simplifies the computation of $\langle x_1 | M | x_s \rangle \equiv \Sigma_j \langle x_1 | e_j \rangle M(j) \langle e_j | x_s \rangle$ and its transpose.

Now relabel the configuration j by the two indices J and α, with J labelling configurations not equivalent to each other under cyclic permutations and α the number of cyclic permutations necessary to obtain j from J. Then because the cyclic permutation operator commutes with T (Kinzel and Schick 1981), the eigenvectors of T satisfy

$$\langle e_{J,\alpha} | x_s \rangle = \exp(2\pi i \alpha p_s / L) \langle e_{J,0} | x_s \rangle \tag{A5}$$

with $0 \leqslant p_s \leqslant L-1$. The partial sums in (A3) then become

$$\begin{aligned}&\sum_{J,\alpha} M(J, \alpha) \langle e_{J,\alpha} | x_s \rangle \langle x_1 | e_{J,0} \rangle \\ &\qquad = \sum_J M(J, 0) \langle e_{J,0} | x_s \rangle \langle x_1 | e_{J,0} \rangle \sum_{\alpha=0}^{\sigma_J - 1} \exp(2\pi\alpha i p_s / L)\end{aligned} \tag{A6}$$

because $p_1 = 0$ and $M(J, \alpha)$ is independent of α; σ_J is the number of configurations equivalent to J (including J). If $\sigma_J p_s / L$ is not an integer then from (A5) $\langle e_{J,0} | x_s \rangle = 0$. If $\sigma_J p_s / L$ is an integer then

$$\sum_{\alpha=0}^{\sigma_J - 1} \exp(2\pi\alpha i p_s / L) = \begin{cases} \sigma_J & p_s = 0 \\ 0 & p_s \neq 0. \end{cases} \tag{A7}$$

Hence, as we stated above, only eigenvectors with $p_s = 0$, i.e. those eigenvectors which are invariant under cyclic permutations of the sites, need to be computed to determine the structure factor in the infinite direction. When the reflection operator commutes with T, similar arguments can be used to reduce the problem further (using $p = 2$, $\exp(i\pi p_s \alpha)$ in (A6) and (A7), with $p_s = 0(1)$ for $|x_s|$ even (odd) under reflection). For spin systems in no magnetic field, as in the present studies, the spin inversion operator commutes with T. Since M is odd under inversion, it is the antisymmetric combination of spin-inversion pairs that contributes, and the delta-function term in (A4) vanishes. The data for $L = 12$ presented in figure 5 required finding all the eigenvalues and eigenvectors of a 102×102 matrix and the largest eigenvalue and its eigenvector for another 122×122 matrix.

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