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LETTER TO THE EDITOR

Finite-size scaling amplitudes in a random tiling model

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Abstract. We study finite-size corrections to the free energy in a two-dimensional random tiling model. This model is equivalent to an asymmetric six-vertex model and exhibits commensurate-incommensurate phase transitions of the Pokrovsky-Talapov type. We calculate finite-size scaling amplitudes of the free energy inside the incommensurate phase, analytically and numerically, by employing a transfer matrix method. Both periodic and free boundary conditions are considered. These amplitudes are consistent with predictions of the theory of conformal invariance with the conformal charge $c = 1$.

Tiling models describing quasicrystals have received a considerable amount of attention recently [1-5]. Experimentally some rapidly quenched alloys were found to have non-crystallographic symmetries with rather sharp diffraction peaks [6]. Recent experiments on AlCuFe [7, 8] revealed diffraction peaks whose width is resolution limited, indicating long range quasiperiodic translational order coexisting with icosahedral bond orientational order. The Penrose tiling, which consists of two types of rhombi tiled together with strong matching rules, is perfectly quasiperiodic and exhibits a Bragg diffraction pattern with a non-crystallographic five-fold symmetry [2]. Penrose tilings and their three-dimensional generalisations are thought to model the quasiperiodic order in quasicrystals.

Random tilings [3] incorporate disorder by loosening the matching rules between tiles. In three dimensions they display Bragg diffraction peaks in addition to a diffuse background. In two dimensions they exhibit quasi-long-range translational order with zero width power law peaks. It is believed that the entropy associated with the random tiling stabilises the quasicrystal phase and favours quasiperiodic translational order. Thus the random tiling scenario and entropic stabilisation are appropriate descriptions of thermodynamically stable quasicrystals. Monte Carlo simulations [9] suggest that equilibrium configurations of certain binary atomic systems at low temperatures are well described as random packings of tiles decorated by atoms with weak matching rules. Experimentally, there are also such strong indications [8, 10]. It is therefore of great interest to study the statistical mechanics of random tiling models.

Recently the transfer matrix method was applied to random tiling models on a semi-infinite strip geometry and was successful in estimating entropies and phason elastic constants in two-dimensional quasicrystal phases [4]. However such calculations suffer from finite-size effects due to the smallness of strip widths attainable with present computers. Moreover, quasicrystal phases in random tiling models are incommensurate phases where an extra length scale (the domain wall separation) is present besides the correlation length (or finite system size) [11]. So one may not blindly use conventional finite-size scaling (FSS) techniques appropriate to systems with only one relevant length scale.

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Park and Widom investigated finite-size effects in incommensurate phases [12, 13]. They showed that the leading finite-size scaling behaviour of the free energy obeys the law of conformal invariance but competition between two length scales generates a deficit (or excess) of domain walls for finite systems with periodic boundary conditions. Due to the presence of this defect, care must be taken in extrapolating finite-size data to bulk values and extracting finite-size scaling behaviour of the free energy. Moreover, with a small number of finite-size data points, extrapolation itself is difficult in general. One principal conclusion of the work presented in this letter is that one can partially overcome the domain wall deficit problem by taking *free* boundary conditions. That is, domain walls can annihilate and/or appear at boundaries. But then one must endure the appearance of non-universal surface terms in the free energy with free boundary conditions. The domain wall deficit problem may still persist in high-order finite-size corrections. In this letter we calculate the FSS amplitudes of the free energy of a random tiling model with periodic and free boundary conditions. Our study serves as the first step towards applying the FSS results to more general random tiling models.

The tiling model we study consists of squares and distorted rhombi (parallelograms) as shown in figure 1. The acute angle of the parallelogram is 45° and lengths of diagonal edges are equal to those of squares. Lengths of horizontal edges of the parallelograms are $\sqrt{2}$ times shorter than the others. These tiles can be put together randomly as long as they do not overlap with each other and there are no gaps between them (figure 2). Then vertices of tiles (including centres of squares) form a square lattice with a lattice

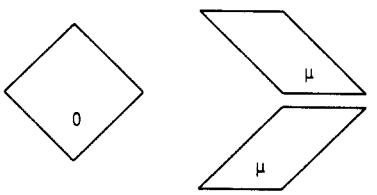

Figure 1. The tiles and their chemical potentials.

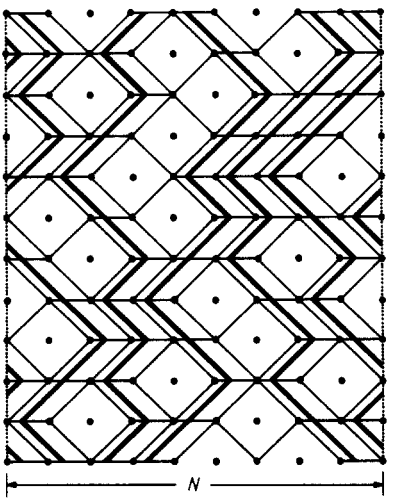

Figure 2. A typical configuration of the tiling model on a semi-infinite strip with strip width $N = 9$. Periodic boundary conditions are imposed. Dots (vertices of tiles and centres of squares) form a square lattice. Bold lines represent domain walls.

constant equal to the length of shorter edges of the parallelograms which we take as our unit of length. We assign the chemical potential μ to a parallelogram and 0 to a square. Varying μ drives the system from the ordered phase of squares to the incommensurate phase. This tiling model is an anisotropic limit of the conventional eight-fold symmetric tiling model [14] for quasicrystals, i.e. 45°-rotated tiles with respect to those in figure 1 are frozen out in our tiling model. In addition, diagonal edges of rhombi and squares are stretched by a factor of $\sqrt{2}$ for convenience. This model is also a distortion of the six-fold symmetric random tiling model [15].

Our tiling model maps onto an asymmetric six-vertex model [16] by one-to-one correspondences between their vertices and edges of tiles (figure 3). Two types of vertices (2 and 3) are frozen out. This model exhibits commensurate-incommensurate phase transitions of the Pokrovsky-Talapov type [17]. One can easily identify domain walls by lines which connect horizontal edges shared by adjoining parallelograms (see figure 2). Note that these domain walls may be recognised as a generalisation of one of the de Bruijn paths of the tilings [18]. These domain walls do not meet each other and their average directions are parallel. On a semi-infinite strip with periodic boundary conditions, the number of parallelograms (or domain walls) per layer n_r is conserved. With strip width N, the number of squares n_s is given by $N = n_r + 2n_s$.

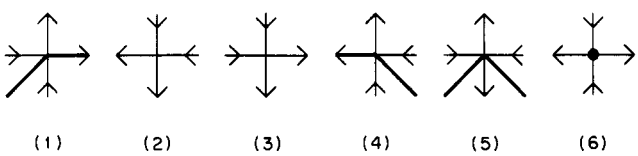

Figure 3. Identifications of edges of tiles with vertices of the six-vertex model. The Boltzmann weights for vertices are given by $\omega_1 = \omega_4 = \exp(\mu)$, $\omega_2 = \omega_3 = 0$, and $\omega_5 = \omega_6 = 1$.

Employing the Bethe-ansatz method, we find the free energy of the finite system under periodic boundary condition, f_N, with n_s squares per layer, is:

$$Nf_N = -\mu n_r - \ln 2 + \frac{1}{2}\sum_{j=1}^{n_s} \ln\left[2 - 2\cos\left(\frac{2j-1-n_s}{N-n_s}\pi\right)\right] \tag{1}$$

for even n_s. We rewrite this equation in a form reminiscent of free fermion models

$$Nf_N = -\sum_{j=1}^{n_r} \ln[2\,e^{\mu}\cos(k_j)] \tag{2}$$

where $k_j = (2j-1-n_r)\pi/N'$ and $N' = N + n_r$. The dispersion relation is $\mathscr{E}(k;\mu) = -\ln[2\,e^{\mu}\cos(k)]$. The distribution of wavevectors k is uniform, which is characteristic of the free fermion model [11]. However, the spacing between nearest-neighbour wavevectors $2\pi/N'$ varies with n_r. So general thermodynamic and finite-size-scaling behaviour must be similar to the free fermion model but certain details are modified.

In the thermodynamic limit, the free energy takes the form

$$f_\infty(k_F;\mu) = \frac{1}{\pi - k_F}\int_0^{k_F} \mathscr{E}(k;\mu)\,dk \tag{3}$$

where the Fermi wavevector $k_F = \lim_{N\to\infty} \pi n_r/N'$. By minimising the free energy with

respect to k_F, we determine the value of k_F for a given μ through the implicit integral equation:

$$f_\infty(k_F;\mu)+\mathscr{E}(k_F;\mu)=0. \tag{4}$$

The thermodynamic behaviour is equivalent to the free fermion model. The dispersion relation has a quadratic shape near $k=0$ and monotonically increases with $|k|$. At $k_F=0$ (or $\mu=-\ln 2$), our model exhibits the Pokrovsky-Talapov transition from the crystal phase with purely squares to the incommensurate critical phase with domain walls. The domain wall density d, defined by $d=\lim_{N\to\infty} n_r/N$, vanishes with critical exponent $\beta=\frac{1}{2}$ as μ approaches μ_c $(=-\ln 2)$ from the side of the incommensurate phase. The specific heat diverges with critical exponent $\alpha=-\frac{1}{2}$. The domain wall density-density correlation function in the incommensurate phase decays algebraically with critical exponent $x=1$.

In this letter, we study finite-size corrections to the free energy inside the incommensurate phase. Finite-size scaling behaviour near the Pokrovsky-Talapov transition will be discussed elsewhere [19]. Finite-size corrections to the free energy may be obtained by applying the Euler-Maclaurin formula to (2). When domain wall densities of finite systems perfectly match the bulk density, i.e. $n_r/N=d$, we find for periodic boundary conditions

$$f_N=f_\infty-\frac{\pi}{6}\frac{\tan(k_F)}{1+d}\Big/N^2+\dots \tag{5}$$

where $k_F=\pi d/(1+d)$. Conformal theory [20, 21] predicts that at criticality the amplitude of $O(1/N^2)$ finite-size corrections to the free energy is $-\frac{1}{6}\pi c\zeta$ for periodic boundary conditions. c is the conformal charge which governs the universality class and ζ is the anisotropy factor equal to the Fermi velocity $\mathscr{E}'(k_F)$. The FSS amplitude in (5) indicates that the conformal charge $c=1$ with the modified anisotropy factor, $\zeta=\mathscr{E}'(k_F)/(1+d)$. The factor $1/(1+d)=N/N'$ results from the unusual wavevector spacing $2\pi/N'$. Later we confirm $c=1$ independently by studying the 90°-rotated geometry.

When domain wall densities of finite systems do not perfectly match the bulk density, the FSS amplitude is modified due to the deficit (or excess) of domain walls in finite systems. The mismatch parameter κ defined by $Nd=n+\kappa$, where n is the integer closest to Nd, represents a deficit of domain walls (see [12]). Perturbation calculations near the perfect density enable us to find the *effective* conformal charge

$$c=1-3\left[\frac{\kappa}{1+d}\right]^2. \tag{6}$$

Note that the effective conformal charge $c=1-3\kappa^2$ for the free fermion model [12]. Again the factor $1/(1+d)$ modifies κ.

Now we repeat the calculation with free boundary conditions. There are no restrictions on tiles at boundaries of the system. We consider a semi-infinite strip geometry with boundaries of not ragged but straight lines. So parts of tiles outside of the strip are cut off (see figure 4). The chemical potential for a fractional tile is taken to be proportional to its area. Domain walls can disappear or reappear at boundaries. The number of domain walls varies layer by layer. So possible values of wavevectors in finite systems are continuous, in contrast to those which are quantised with periodic boundary conditions. Therefore finite systems with free boundary conditions find a

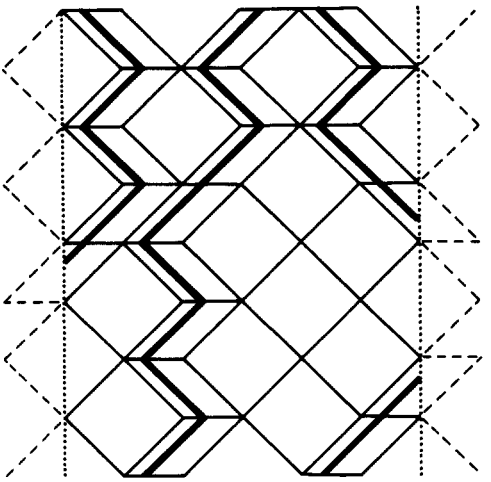

Figure 4. A typical configuration of the tiling model with free boundary conditions. Parts of tiles outside of the strip are cut off. Notice that domain walls (bold lines) can disappear and/or reappear at boundaries.

true ground state where there is no excess (or deficit) of domain walls†. Notice that these boundary conditions are completely different from the conventional free boundary conditions in quantum spin chain models [22], where the number of domain walls is still a good quantum number so there are still κ effects.

There are no exact solutions available for finite systems with free boundary conditions. We calculate the free energy numerically on a semi-infinite strip using transfer matrix techniques. As usual the system is divided into layers. A state of a layer is determined by positions of squares; $X=\{x_1, x_2, \ldots, x_{n_s}\}$ where x_i is the position of the centre of the ith square. Except for those closest to boundaries, each square of a given layer must be located in between neighbouring squares of the neighbouring layer

$$x_1 < y_1 < x_2 < y_2 < \ldots \qquad \text{or} \qquad y_1 < x_1 < y_2 < x_2 < \ldots \tag{7}$$

where $Y=\{y_1, y_2, \ldots, y_{n_s'}\}$ represents the positions of centres of squares of the neighbouring layer. With free boundary conditions the number of centres of squares can vary layer by layer and its variance between neighbouring layers is $n_s - n_s' = 0, \pm 1$. Note that centres of squares at the boundaries contribute fully to n_s and n_s' even though they only contribute as half squares to the chemical potential.

The transfer matrix, $\mathcal{T}(X, Y)$, is very sparse. Most matrix elements are zero because of the above condition (7). Exploiting the sparsity to reduce computer storage, we can study a system with a relatively large strip width ($N=17$). We calculate the largest eigenvalue Λ of the transfer matrix with system sizes N from 1 up to 17. The free energy of the system is given by $f=-(\ln \Lambda)/N$. We assume that the form of finite-size corrections is $f_N = f_\infty + f_s/N - A^f/N^2 + \ldots$. Conformal theory predicts $A^f = \frac{1}{24}\pi c\zeta$ for

† With free boundary conditions, the domain wall density in finite systems is not the same as the bulk density but has a $O(1/N)$ correction. This correction results entirely from the surface free energy f_s, i.e. $\mathrm{d}f_s/\mathrm{d}\mu$. In contrast, the system with periodic boundary conditions is forced to have a deficit (or excess) of domain walls with no surface free energy. So with free boundary conditions the system has no excess (or deficit) of domain walls in viewpoint of the true ground state where there are no domain walls forced into (or out of) the system. Only these forced ones contribute to the finite-size scaling amplitude of the $O(1/N^2)$ term of the free energy.

free (or fixed) boundary conditions [20, 21]. The bulk free energy f_∞ is exactly known from (3) and (4). Fitting our numerical data into the above form yields a sequence of $A_N^{\mathrm{f}} \equiv N(N+1)[(N+1)f_{N+1} - Nf_N - f_\infty]$ $(N = 1, 2, \ldots, 16)$. This sequence is then extrapolated to the thermodynamic limit using the θ algorithm [23].

We carry out our calculations for $-0.6 \leqslant \mu \leqslant 0.4$ inside the incommensurate phase. Table 1 displays a sampling of numerical values of $4A_N^{\mathrm{f}}/A^{\mathrm{p}}$ at several values of μ where $A^{\mathrm{p}} = \pi\zeta/6$ is the FSS amplitude for periodic boundary conditions, see (5). Conformal theory predicts that this ratio is 1 [21]. Extrapolated values of this ratio are close to 1 (within 1% error) in most regions. Notice that these ratios change drastically near $\mu = \mu_{\mathrm{c}} = -\ln 2$ where anisotropic scaling sets in (the anisotropy factor $\zeta \to 0$) so the conformal invariance disappears [11]. This anisotropic finite-size scaling behaviour will be discussed elsewhere [19].

Table 1. The ratio of finite-size scaling amplitudes of the free energies with free and periodic boundary conditions multiplied by a factor of 4; $4A_N^{\mathrm{f}}/A^{\mathrm{p}}$. We list finite-size data for several values of strip width N and chemical potential μ. The values in the last row are extrapolations to the thermodynamic limit using the θ algorithm. At $\mu = -0.6$ the θ algorithm fails and the extrapolated value depends on extrapolation techniques.

$4A_N^{\mathrm{f}}/A^{\mathrm{p}}$	$\mu = -0.6$	-0.4	-0.2	0.0	0.2	0.4
$N = 8$	1.463 24	1.035 87	0.875 11	0.744 94	0.619 95	0.619 95
10	1.332 61	1.026 47	0.895 74	0.895 73	0.673 97	0.559 02
12	1.257 28	1.020 02	0.910 20	0.813 73	0.714 19	0.607 78
14	1.224 93	1.015 87	0.921 02	0.835 59	0.745 39	0.646 64
16	1.186 26	1.012 86	0.929 47	0.852 79	0.770 37	0.678 39
∞	1.210 48	1.010 22	1.005 96	1.005 39	1.011 34	1.015 56

Finally we present the numerical results on the 90°-rotated geometry with periodic boundary conditions. On these strips domain walls lie perpendicular to the direction of the infinite dimension. There are no κ effects since there is no discreteness in the finite-size domain wall density. However, with odd N (strip width), the system cannot have equal numbers of right- and left-tilting parallelograms in a layer. This means that directions of the domain walls are slightly tilted with respect to the horizontal direction. The broken symmetry between two kinds of parallelograms would generate an extra term in the FSS amplitude of the free energy.

When N is even, the symmetry between two kinds of parallelograms is maintained. In this letter we study the system with even N only, up to $N = 12$. We use periodic boundary conditions to remove surface terms in finite-size corrections to the free energy. Finite-size data for the free energy are fitted into the form; $f_N = f_\infty - A^{\mathrm{r}}/N^2 + \ldots$. As in the previous case, we find a sequence $\{A_N^{\mathrm{r}}\}$. Extrapolated values of the FSS amplitudes are obtained again by using the θ algorithm. The product of two FSS amplitudes, $A^{\mathrm{p}}A^{\mathrm{r}}$, in two orthogonal geometries cancels the anisotropy factor and takes the value $(\pi c/6)^2$ [24]. Table 2 displays a sampling of numerical values of $c_N \equiv (6/\pi)\sqrt{A^{\mathrm{p}}A_N^{\mathrm{r}}}$ at several values of μ. Extrapolations of c_N to the bulk should yield the value of the conformal charge c. In most regions, except near $\mu = \mu_{\mathrm{c}}$, the conformal charge c is very close to 1 (within 0.2% error). This confirms our previous identification of the anisotropy factor $\zeta = \mathscr{E}'(k_{\mathrm{F}})/(1+d)$ and the conformal charge $c = 1$.

Table 2. Approximations to the conformal charge, c_N. We list finite-size data for several values of strip width N and chemical potential μ. The values in the last row are extrapolations to the thermodynamic limit using the θ algorithm. At $\mu = -0.6$ the θ algorithm fails and the extrapolated value depends on extrapolation techniques.

c_N	$\mu = -0.6$	-0.4	-0.2	0.0	0.2	0.4
$N = 4$	0.570 25	0.975 33	1.099 67	1.115 01	1.101 73	1.088 27
6	0.704 58	1.065 40	1.087 96	1.060 95	1.043 30	1.035 56
8	0.805 96	1.085 22	1.058 17	1.032 47	1.022 52	1.019 04
10	0.883 25	1.078 53	1.037 12	1.019 40	1.013 84	1.011 94
12	0.941 90	1.064 60	1.024 53	1.012 88	1.009 42	1.008 21
∞	1.173 82	1.060 70	1.002 22	0.998 75	0.998 32	0.998 07

In summary, we have studied a random tiling model and found a commensurate-incommensurate phase transition between a crystal phase of squares and an incommensurate critical phase. The finite-size corrections to the free energy inside the incommensurate phase are similar to those of the free fermion model. Analytic and numerical calculations show that the FSS amplitudes of the free energies are consistent with predictions by the conformal theory with the conformal charge $c = 1$.

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