Finite-Size-Scaling Amplitudes of the Incommensurate Phase

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We examine the finite-size-scaling amplitudes of the free energy in incommensurate phases on a torus with periodic and twisted boundary conditions. We show that these amplitudes are equivalent to those of the six-vertex model with electric and magnetic defect lines. The twist angle generates magnetic defect lines, while the electric defect lines are generated by competition between the domain-wall separation and the finite system size. We calculate the amplitudes exactly for the free-fermion model and the spin-$\frac{1}{2}$ *XXZ* chain, and conjecture the form of these amplitudes for a more general model. Numerical calculations employing the Bethe *Ansatz* confirm our conjecture.

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The discovery that many two-dimensional critical systems are conformally invariant gives much insight into their critical behavior.[1] All information about critical exponents and universal behavior is contained in the conformal charge c and the operator content. Conformal invariance relates the universality class of a system to the finite-size corrections to the free energy.[2-4] This relation has been applied successfully to two-dimensional models on strips of finite widths employing the transfer-matrix method[5] and also on finite-by-finite lattices employing Monte Carlo simulations.[6] Unfortunately, it is not easy to know *a priori* which conformal charge is associated with a given system or indeed whether conformal invariance is present at all.

In this Letter, we investigate the finite-size-scaling (FSS) amplitudes of the free energy in two-dimensional incommensurate phases.[7] Numerical data for the FSS amplitudes in incommensurate phases appear superficially as if they do not converge in the thermodynamic limit[8-10] [see Fig. 1(a)]. The apparently random behavior of the FSS amplitudes makes it difficult to get any information about the critical exponents from FSS behavior of the free energy in incommensurate phases, in contrast to ordinary phases. We explain why these amplitudes are scattered and present a systematic way of analyzing the data.

The incommensurate phase is a critical phase with a continuously varying domain-wall density d. Domain-wall density correlation functions decay algebraically with a modulation such that domain walls are placed at distances $l=1/d$ on average. The critical index of the domain-wall density, x, varies continuously with incommensurability. The existence of an extra length scale (the domain-wall separation l) raises some concerns about the conformal invariance of the incommensurate phase.[9-11] We show that competition between the domain-wall separation and the system size introduces electric defect lines but leaves conformal invariance intact.

Previously we investigated the FSS behavior in the

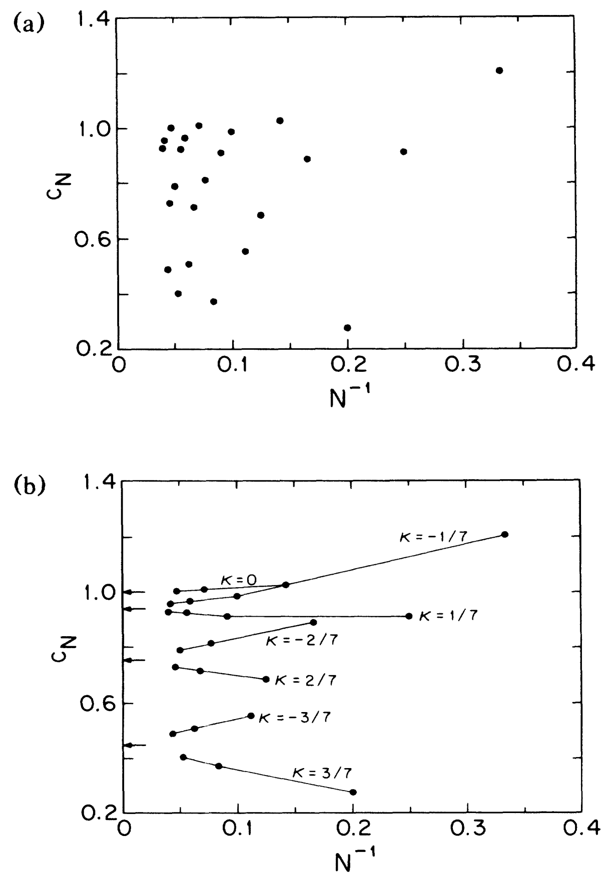

FIG. 1. (a) Numerical data for the FSS amplitudes of the free-fermion model for the domain-wall density $d=\frac{2}{7}$ on an infinite cylinder of width N with periodic boundary conditions. c_N is proportional to the FSS amplitudes; $c_N=(6/\pi\zeta)N^2(f_\infty-f_N)$, where ζ is the anisotropy factor. f_N is the exactly known ground-state energy for finite systems (Refs. 7 and 10) and f_∞ is the bulk term. (b) Classification of numerical data for different values of mismatch parameter κ. Arrows indicate the exact values of the conformal charge c_∞ obtained from Eq. (6). Lines between data points are only guides to the eye.

free-fermion model,[10]

$$\mathcal{H}_{\rm FF}=m\sum_{n=1}^{N}\sigma_n^+\sigma_n^- -\frac{t}{2}\sum_{n=1}^{N}(\sigma_n^+\sigma_{n+1}^- +\sigma_n^-\sigma_{n+1}^+)\,, \quad (1)$$

and found an unusual boundary effect arising from mismatch between system size and domain-wall separation. On discrete lattices, the FSS amplitudes depend on how well the lattice size (N) matches an integral multiple of the domain-wall separation l. Since the number of domain walls present in a system with periodic boundary conditions is always an integer, the density in finite systems rarely matches the bulk density d exactly. Thus there is almost always a deficit (or excess) of domain walls in finite systems. We introduce a mismatch parameter κ defined by $Nd=n+\kappa$ (n is the integer closest to Nd and $-\frac{1}{2}<\kappa\le\frac{1}{2}$). The value of n is the number of domain walls in the ground state of the finite system, so κ represents the deficit of domain walls. Figures 1(a) and 1(b) show how this mismatch influences the FSS amplitudes. The amplitudes obey the laws of conformal invariance, but with conformal charge altered by missing domain walls.

Recently the FSS spectrum of the spin-$\frac{1}{2}$ XXZ Heisenberg chain,

$$\mathcal{H}_{XXZ}=-\tfrac{1}{2}\sum_{n=1}^{N}[\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y+\Delta\sigma_n^z\sigma_{n+1}^z]\,, \quad (2)$$

has been studied extensively by several authors,[12-14] using the conformal theory and the Bethe *Ansatz* method. Its operator content is explored for various boundary conditions. Twisted boundary conditions $[\sigma_{N+1}^{\pm}=\sigma_1^{\pm}\times\exp(\pm i2\pi\phi)]$ connect the operator content of the XXZ chain to those of some other models like the q-state Potts models.[13,14] The twist angle ϕ generates magnetic defect lines in the Coulomb-gas language.[15]

This paper considers a model which combines the chemical potential m (or magnetic field) of the domain walls in the free-fermion model with the domain-wall interaction Δ of the XXZ chain;[9,11]

$$\mathcal{H}=\mathcal{H}_{XXZ}+m\sum_{n=1}^{N}\sigma_n^+\sigma_n^-\,. \quad (3)$$

The chemical potential m controls the domain-wall density d. For the ordinary XXZ chain[16] ($m=0$), there is no net polarization in the critical phase ($-1<\Delta<1$), i.e., $d=\frac{1}{2}$. This model with variable domain-wall density is a quantum-mechanical prototype for physically relevant incommensurate solid phases such as occur in the chiral three-state Potts model and the axial next-nearest-neighbor Ising model in two dimensions (for a review, see Ref. 7). The effect of dislocations on the FSS amplitude is not studied here.

We carry out our analysis on a torus of length M in the temporal direction (parallel to domain walls) and width N. The partition function of the domain-wall system on an $N\times M$ lattice with periodic boundary conditions in the vertical (temporal) direction is

$$Z=\mathrm{Tr}\exp(-M\mathcal{H})\,. \quad (4)$$

In the infinite-cylinder limit ($M\to\infty$), we show that the finite-size corrections to the free energy (log of the partition function) of the free-fermion model and the XXZ chain take the form

$$f_N=f_\infty-(\pi/6)\zeta c/N^2+\cdots\,, \quad (5)$$

where ζ is the anisotropy factor and c, the conformal charge, is given by

$$c=1-6\left[\frac{K_G}{2\pi}\kappa^2+\frac{2\pi}{K_G}\phi^2\right]. \quad (6)$$

K_G is the Gaussian coupling constant related to the correlation-function critical exponent x by $K_G=\pi x$.[4] The exponent x is always 1 for the free-fermion model, independent of the value of the domain-wall density. For the XXZ chain, the mismatch parameter $\kappa=0$ ($\frac{1}{2}$) for even (odd) N because the ground-state domain-wall density d is always $\frac{1}{2}$. In the model defined by Eq. (3), both x and κ vary continuously with the domain-wall density d.[11,17] The exponent x also varies with the strength of domain-wall interactions Δ. We find that the form of the finite-size corrections in Eqs. (5) and (6) remains unchanged in this model. The mismatch parameter κ controls the strength of the electric defect line in the Coulomb gas, while the angle ϕ in twisted boundary conditions controls the magnetic defect line.[15] Notice that κ plays a similar role to the twist angle angle in *vectorlike* twisted boundary conditions[15] at $d=\frac{1}{2}$.

Consider first the free-fermion model. The dispersion relation $\mathcal{E}(k)=m-t\cos(k)$ in this model. However, our final results depend only on a few of the general properties of the dispersion relation.[10] We analyze the partition function by an asymptotic expansion method used by several authors for Ising and dimer models.[8,18] Applying this technique to the free-fermion model,[10] it is straightforward to obtain the leading finite-size corrections to the partition function. First, we introduce some parameters: the aspect ratio $s=M/N$; the Fermi wave vector k_F satisfying $\mathcal{E}(k_F)=0$; the domain-wall density $d=k_F/\pi$; and the anisotropy factor (Fermi velocity) $\zeta=\mathcal{E}'(k_F)$. The partition function, up to the $O(1)$ term, takes the form

$$Z(\kappa,\phi)\simeq\exp(-MNf_\infty)\frac{q^{\kappa^2/2+2\phi^2}}{2\eta^2(q)}\sum_{i=1}^{4}p_i\theta_i\left[\frac{z_\kappa}{2}+z_\phi,q\right]\theta_i\left[\frac{z_\kappa}{2}-z_\phi,q\right], \quad (7)$$

where $q=\exp(-\pi s\zeta)$, $p_1=-1$ and $p_i=1$ for $i=2,3,4$, $z_\kappa=i\pi s\zeta\kappa$, $z_\phi=i\pi s\zeta\phi$, θ_i is the Jacobi's theta function of the ith kind, and η is the Dedekind eta function.[4,19]

Note that $\exp(-MNf_\infty)$ is the bulk term in the partition function, while its coefficient is the $O(1)$ term. The form of the $O(1)$ term in the partition function is universal. The only model dependence enters through the anisotropy factor ζ which modifies the aspect ratio by $s\to s\zeta$ as usual for anisotropic systems in the conformal theory.[1] At $\phi=0$ (periodic boundary conditions), the same formula has been obtained by Bhattacharjee for the generalized dimer model.[8] We observe that the $O(1)$ part of the partition function simplifies to

$$Z^{O(1)}(\kappa,\phi)=\frac{q^{\kappa^2/2+2\phi^2}}{\eta^2(q)}\theta_3\left(\frac{z_\kappa}{2},q^{1/2}\right)\theta_3(2z_\phi,q^2). \quad (8)$$

This expression is similar to $Z^{O(1)}$ of the six-vertex model (or the Coulomb gas).[4,20] In fact, when $\kappa=\phi=0$, Eq. (8) becomes identical to $Z^{O(1)}$ of the six-vertex model at the free-fermion point ($\Delta=0$) with periodic boundary conditions, aspect ratio $s\zeta$, and an even number of sites.[4]

Using the definition of the θ function[4,19] we rewrite the above equation in a form reminiscent of the Coulomb-gas partition function

$$Z^{O(1)}(\kappa,\phi)=\frac{1}{\eta^2(q)}\sum_{e,m\in Z}q^{(1/2)(e-\kappa)^2+2(m-\phi)^2}, \quad (9)$$

where e and m are integers and called the electric and magnetic charge, respectively, in the Coulomb-gas language.[21] So κ and ϕ represent the electric and magnetic defect in the Coulomb-gas system. The partition function of the Coulomb gas (or the six-vertex model) parametrized by the Gaussian coupling constant K_G is[4]

$$Z_{CG}^{O(1)}=\frac{1}{\eta^2(q)}\sum_{e,m\in Z}q^{(K_G/2\pi)e^2+(2\pi/K_G)m^2}. \quad (10)$$

The six-vertex parameters Δ and K_G are related by $\Delta=-\cos(\mu)$ and $K_G=2(\pi-\mu)$.[16]

By comparing our result Eq. (9) with the Coulomb-gas form Eq. (10), it is tempting to generalize Eq. (9) off the free-fermion point (i.e., to nonzero Δ)

$$Z^{O(1)}(\kappa,\phi)=\frac{1}{\eta^2(q)}\sum_{e,m\in Z}q^{(K_G/2\pi)(e-\kappa)^2+(2\pi/K_G)(m-\phi)^2}. \quad (11)$$

At $\Delta=0$, $K_G=\pi$ and we recover our free-fermion result in Eq. (9). Taking the infinite-cylinder limit ($s\to\infty$) reveals the finite-size behavior in Eqs. (5) and (6). This form has been already shown to be correct for the XXZ chain at $d=\frac{1}{2}$ numerically[14] and analytically.[13] We conjecture that Eq. (11) remains correct in the more general model [Eq. (3)] where the Gaussian coupling constant K_G is still given by πx but x now depends on both Δ and d.

The free-energy difference between when $\kappa=0$ and nonzero κ represents the free energy of the κ missing domain walls. So κ plays the same role as steps in step boundary conditions in the body-centered solid-on-solid or the Gaussian model,[4] where the height at the site $N+1$ is lower by κ than at the site 1. This relation is also apparent in the six-vertex model. The net polarization in the horizontal direction, P_1 [see Eq. (4.9) in Ref. 4], represents the number of up arrows which can be identified by domain walls. The number of missing domain walls κ corresponds to the shift of the net polarization P_1 from integer values by κ. Since P_1 corresponds to the electric charge in the Coulomb-gas formalism, this shift in P_1 is identical to an electric defect in the Coulomb-gas system. Hamer and Batchelor[13] recently observed this effect in the XXZ chain. By investigating the energy spectrum of the $d=\frac{1}{2}$ sector with extra domain walls, they found that the free energy with n extra domain walls is given by Eqs. (5) and (6) after replacing κ by n.

It is interesting to perform an inversion transformation on Eq. (8) using Jacobi's inversion formulas for θ functions.[19] The partition function becomes

$$Z^{O(1)}(\kappa,\phi)=\frac{1}{\eta^2(\tilde{q})}\theta_3(\tilde{z}_\phi,\tilde{q}^{1/2})\theta_3(\tilde{z}_\kappa,\tilde{q}^2), \quad (12)$$

where $\tilde{q}=\exp(-\pi/s\zeta)$, $\tilde{z}_\kappa=\pi\kappa$, and $\tilde{z}_\phi=\pi\phi$. The aspect-ratio $s\to 0$ limit is especially simple in Eq. (12). Expanding the free energy for small $\tilde{q}$ in the above equation, we find

$$f(\kappa,\phi)=f_\infty-\frac{\pi/6\zeta}{M^2}+\cdots. \quad (13)$$

There is no discreteness in the domain-wall density in this geometry because the domain walls lie perpendicular to the infinite-cylinder direction. Therefore the κ-dependent term disappears. The twisted boundary conditions in the infinite-cylinder direction also do not contribute to the finite-size corrections of the free energy. As usual in conformally invariant systems, the anisotropy factor ζ in the FSS amplitude is placed in the denominator, in contrast to the orthogonal cylinder geometry in which ζ appears in the numerator.

We tested our conjecture through Bethe *Ansatz* calculations. The extra mass term in Eq. (3) does not alter the Bethe *Ansatz* equations for allowed wave vectors, so we solve precisely the same equations as in Refs. 13 and 14. Because we are interested in moving the ground-state domain-wall density d away from the value $\frac{1}{2}$ at which exact solutions are known,[16] we solve the equations numerically in general, and perturbatively in certain limits. The form of the FSS amplitude in Eqs. (5) and (6) agrees with our numerical calculations for several different values of Δ and d. In particular, we show that the FSS amplitudes contain no dependence on κ or ϕ other than quadratic terms, there are no cross terms, and that the coefficients of κ and ϕ have an inverse relation. Table I displays a sampling of numerical values of $x=K_G/\pi$ obtained from our calculations.

TABLE I. Numerical values of correlation-function critical exponents $x = K_G/\pi$ for several different values of $\mu = \cos^{-1}(-\Delta)$ and domain-wall density d.

$x(\mu,d)$	$d=\frac{1}{2}$	$d=\frac{1}{3}$	$d=\frac{1}{4}$	$d=\frac{1}{5}$	$d=0$
$\mu=\pi/2$	1	1	1	1	1
$\mu=\pi/3$	$\frac{4}{3}$	1.2474	1.1839	1.1451	1
$\mu=\pi/6$	$\frac{5}{3}$	1.3938	1.2780	1.2143	1
$\mu=0$	2	1.4404	1.3062	1.2346	1

Note that $x=2(\pi-\mu)/\pi$ for the XXZ chain at $d=\frac{1}{2}$. Expansion away from the free-fermion model ($\Delta \simeq 0$) yields

$$x = 1 - 2\Delta \frac{\sin(\pi d)}{\pi} + \cdots \tag{14}$$

for arbitrary d. For arbitrary Δ we obtain

$$x = 1 - \frac{2\Delta}{1-\Delta} d + \cdots \tag{15}$$

in the small-d limit. Notice that x takes the free-fermion value 1 in the $d=0$ limit in addition to the obvious $\Delta=0$ limit.

In summary, we study a general model of the incommensurate phase in two dimensions consisting of interacting fermions. We show that ideas of conformal invariance do indeed apply to the incommensurate phase. In addition, we conjecture that Eq. (11) describes FSS amplitudes on a torus. We confirm the conjecture in the infinite-cylinder limit through numerical Bethe *Ansatz* calculations and perturbation theory. Our model can actually be mapped onto the six-vertex and Gaussian models. Twisted boundary conditions generate magnetic defect lines, while mismatch between the domain-wall spacing l and the system size N creates electric defect lines.

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