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Critical properties of two-dimensional models

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Critical properties of two-dimensional classical models and (1 + 1)-dimensional quantum models are obtained by solving a general dimerized spin chain. The staggered-electric exponent of the F model is derived. The central role of umklapp scattering in controlling renormalization and determining Potts-model critical exponents is pointed out. The thermal exponent of the Potts model is evaluated, and the validity of den Nijs conjecture is established. Logarithmic singularities at the multicritical point are obtained.

It is widely recognized that there is a close connection between the critical properties of a great many models in two space or space-time dimensions. The general classical problem may be stated as an eight-vertex model with both staggered and direct fields, which contains the Baxter and staggered-F models as special cases and may be mapped exactly into the Ising, Potts, Ashkin-Teller,[1] and body-centered-solid-on-solid roughening models.[2] Its transfer matrix[3] is related to a dimerized quantum spin chain (XYZ model) and to the equivalent spinless Fermi gas. Furthermore, in the scaling limit, systems of classical charges, planar spins, fermions with spin, sine-Gordon bosons, and general roughening models may be fitted into the same picture.[4] These models are encountered in a wide variety of physical situations, particularly adsorbed films, organic conductors, ice-rule ferroelectrics, and magnetic materials.

The purpose of this Communication is to give a unified derivation of the critical properties of these systems, extending an approach first introduced by Luther and Peschel[5] for the uniform Baxter model, and further developed by Kadanoff and Brown.[6] We shall work with the fermion representation of the transfer matrix and show that, in order to obtain a complete picture, incorporating the crossover to a new phase at the end of the fixed line, it is necessary to recognize the importance of umklapp scattering, and to follow explicitly the renormalization from the bare Hamiltonian to the neighborhood of the fixed line. In particular, we shall determine the complete temperature dependence of the staggered-field exponent of the F model, and give a derivation of the thermal exponents of the Potts models,[1,7] showing the importance of a delicate cancellation of the leading singularities.

Our approach makes use of Temperley and Lieb's device of a transfer matrix which builds up a lattice diagonally.[3] In Hamiltonian form[8] ($T \rightarrow e^{-H}$) it may be written in terms of fermion variables as $H = H_0 + tH_1$ where

$$H_0 = -\sum_{n=1}^{2M} (K_n - 2g\rho_n\rho_{n+1}) \ , \tag{1}$$

$$H_1 = -\sum_{n=1}^{2M} (-1)^n (D_1K_n + D_2\rho_n\rho_{n+1} + D_3\rho_n) - B\sum_{n=1}^{2M} (a_n^\dagger a_{n+1}^\dagger + a_{n+1}a_n) \ . \tag{2}$$

Here $K_n \equiv a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n$, $\rho_n \equiv a_n^\dagger a_n$, and the parameter t is proportional to the staggered field for the F model and to $T - T_c$ for other classical systems. Table I gives the values of g, D_i, and B at $t = 0$ for the different models. Critical properties are obtained from the ground state of H, and, for $|g| \leq 1$, H_0 has power-law correlation functions corresponding to a line of critical points with variable exponents.

Asymptotic forms of correlation functions may be studied by introducing a lattice spacing $s = L/2M$ and taking the continuum limit $s \rightarrow 0$ by letting $M \rightarrow \infty$ with L fixed. Then it is necessary to have $m \rightarrow \infty$ if the coordinate $x = 2ms$ remains finite as $M \rightarrow \infty$. Introducing right- and left-going field operators[4] $\psi_1(x) = (-1)^m(\psi_{2m} - i\psi_{2m+1})/2s^{1/2}$ and $\psi_2(x) = (-1)^m(\psi_{2m} + i\psi_{2m+1})/2s^{1/2}$, and replacing sums

TABLE I. Values of the coefficients D_i, B, and g for different models. The notation $\tilde{g}=i(1-g^2)^{1/2}$ and $r=(1+2g)(1+g)\ln(1+2g)/2g$ has been used. K is the four-spin interaction of the Ashkin-Teller model and a is a vertex weight.

Model	$(g+\frac{1}{2})D_1$	$(g+\frac{1}{2})D_2$	$(g+\frac{1}{2})D_3$	B	g
Potts	1	$-2g$	$2\tilde{g}$	0	$q^{1/2}/2$
Ashkin-Teller	$\frac{1+g-r(1-g)}{2g^2}$	$-2g$	$\frac{\tilde{g}[(1+g)^2-r]}{g^2(1+g)}$	0	$\frac{1}{2}\coth^2 K/2-1$
Staggered F	$\frac{\tilde{g}(1+2g-r)}{2g^2}$	0	$\frac{(g^2-1)(1+2g)+r}{g^2}$	0	$\frac{1}{2}4^{T_c/T}-1$
Baxter	0	0	0	$2^{1/2}(1+g)^{1/2}$	$\frac{1}{2}a^{-2}-1$

over m by integrals over x, we obtain

$$\frac{MH_0}{L}=\int_0^L dx\left[i\left(\psi_1^\dagger\frac{\partial\psi_1}{\partial x}-\psi_2^\dagger\frac{\partial\psi_2}{\partial x}\right)+g_D(\rho_1^2+\rho_2^2)+8g_D\rho_1\rho_2+g_u(R_1^\dagger R_2+R_2^\dagger R_1)\right], \quad (3)$$

$$H_1=-\int_0^L dx\,[D^+\psi_2^\dagger\psi_1+D^-\psi_1^\dagger\psi_2+\overline{B}(\psi_1^\dagger\psi_2^\dagger+\psi_2\psi_1)], \quad (4)$$

where $\rho_i(x)\equiv\psi_i^\dagger(x)\psi_i(x)$, $R_i\equiv\psi_i(x-2s)\psi_i(x)$, $D^\pm\equiv\pm 2i(\overline{D}_1-\overline{D}_2/\pi)-\overline{D}_3$. Renormalized coupling constants for direct and umklapp scattering, dimerization, and the thermal perturbation of the Baxter model are denoted by g_D, g_u, $\overline{D}_i$, and $\overline{B}$, respectively, and they will be determined from renormalization-group equations, which are most conveniently derived by rewriting the problem in Coulomb-gas language. This may be accomplished by making a boson representation of the fermion operators in Eqs. (3) and (4), thereby transforming H into a multiple sine-Gordon Hamiltonian and enabling us to carry out an explicit expansion of $\mathrm{Tr}\exp(-2MH)$ in powers of g_u, $D^\pm$, and $\overline{B}$. The resulting series is the grand partition function of a Coulomb gas which has two types of mutually interacting charges with fugacities g_u and $D^\pm$, and a third, independent, set of charges with fugacity $\overline{B}$. Given this representation, it is well known[4,9,10] how to write down renormalization-group equations as expansions in the fugacities:

$$\frac{d\theta}{dl}=\frac{1}{2}y^2, \quad (5)$$

$$\frac{dy}{dl}=\left(2-\frac{2}{\theta}\right)y, \quad (6)$$

$$\frac{dD^\pm}{dl}=\left(2-\frac{1}{2\theta}\right)D^\pm-\frac{1}{2}yD^\mp, \quad (7)$$

$$\frac{d\overline{B}}{dl}=(2-2\theta)\overline{B}. \quad (8)$$

Here y is proportional to g_u, θ is a function of g_D, and $l\equiv\ln M$ (note that $L/2M$ is the lattice spacing). The variables $D^\pm$ do not appear on the right-hand side of Eqs. (5) and (6), since their effect can always be made negligible by starting with weaker fields or smaller deviations from T_c. Consequently Eqs. (5) and (6) are the renormalization-group equations for a single Coulomb gas, and they may be solved independently for $\theta(l)$ and $y(l)$. The scaling trajectories are well known,[4,9,10] and they are shown in Fig. 18 of Ref. 10 (with $2/\theta\to\pi K$). Asymptotically, for $g<1$, $y\to 0$ and θ tends to a fixed-point value $\theta_0(g)$ that is determined by the boundary conditions. Once $\theta(l)$ and $y(l)$ are known, Eqs. (7) and (8) may be solved for $D^\pm$ and $\overline{B}$, to obtain the critical behavior.

Equations (5)–(8) are not valid for the whole trajectory, since the starting value of y is not small for all g. Furthermore, although t is small, it is necessary to follow the evolution of the D_i from the starting values shown in Table I to the asymptotic forms that make up $D^\pm$. This is of particular importance for the Potts models. For these reasons, we have carried out the early stages of renormalization numerically by studying the M dependence of the energy levels[11] of H, obtained by diagonalizing the matrix for lattices of size $2M\leq 16$. These numerical results were matched onto the analytical solutions of Eqs. (4) and (5), in the domain where both are valid. This procedure is tantamount to a numerical evaluation of θ_0, and the results are in agreement with the expression

$$\cos\pi(1-\theta_0)=g \quad (9)$$

obtained from the exactly known thermal eigenvalue of the Baxter model.[12,13] However we have also verified it for the quite different form of thermal perturbation that leads to Eq. (7). Once this global connection between θ_0 and g has been established, it is possible to use Eqs. (5)–(7) to obtain corresponding exponents for other models.

By now it is clear that umklapp scattering plays exactly the same role as vortices in the planar model,[9,10] which is asymptotically equivalent[2,14] to H_0. This process was omitted by Luther and Peschel,[5] who were the first to discuss the continuum form of the uniform Baxter model and spin chain ($D_i = 0$). Thus their calculation is analogous to Berezinskii's original spin-wave theory[15] of the planar model, and it misses the analog of the vortex unbinding transition[9,10] to a phase with finite coherence length ξ, in the region $g > 1$ ($\theta_0 > 1$) where umklapp scattering is a relevant perturbation.

For $g > 1$, the analytical form of ξ may be obtained by replacing Eq. (9) with $\cosh\lambda = g$. The scaling trajectories then pass through $y = y_0 \equiv 2\lambda/\pi$ for $\theta = 1$, and, using Kosterlitz's result[9] $\xi \sim \exp(\pi/y_0)$, we find

$$\xi \sim \exp(\pi^2/2\lambda) \tag{10}$$

in agreement with the exact result of Johnson, Krinsky, and McCoy.[13] Alternatively, Eq. (10), together with $\cosh\lambda = g$, could have been used as a starting point to derive Eq. (9).

We now apply these results to the F model with a staggered-electric field, conjugate to the antiferroelectric order parameter. Variations in temperature correspond to changes in g, and the value $g = 1$ ($\theta_0 = 1$) marks the phase transition in zero field first elucidated by Lieb.[16] In our picture this is an umklapp-driven transition. Its relationship to the plasma-insulator transition of the Coulomb gas was already evident from the work of van Beijeren[2] and Chui and Weeks.[17] If s is the staggered field, and $T > T_c$ (i.e., $-\frac{1}{2} \leq g < 1$), Eq. (7) and the renormalization-group equation for the free energy show that there is a singular contribution to the F-model free energy of the form $f \sim |s|^{2/y_s^F}$, where $y_s^F = 2 - (2\theta_0)^{-1}$. This defines the staggered-electric exponents $\eta = 4 - 2y_s^F$ and $\delta = (4 - \eta)/\eta$ which are temperature dependent, with η ranging from 1 at $T = T_c$ to 3 as $T \rightarrow \infty$. Our result agrees with the exact values[18] $\eta = 2$, $\delta = 1$ at $T = 2T_c$, and is (to our knowledge) the first derivation of the complete T dependence of these exponents. The value of y_s^F is experimentally accessible, and it has been measured[19] in stannous chloride dihydrate giving $\frac{4}{3} \lesssim \eta \lesssim \frac{3}{2}$. Unfortunately, the magnitude of T/T_c was imprecisely known, and it would be of interest to carry out further experiments to see if the temperature dependence of η is consistent with our results.

A similar discussion may be given for the Ashkin-Teller model, for which our whole picture is consistent with the general point of view developed by Kadanoff in a series of publications.[6,20,21] For $-\frac{1}{2} \leq g \leq 1$, Eqs. (7) and (9) together with Table I show that the singular part of the free energy goes as $f \sim |t|^{2/y_T^{\mathrm{AT}}}$ with $t \sim T - T_c$, $y_T^{\mathrm{AT}} = 2 - (2\theta_0)^{-1}$, and $\sin(\pi\theta_0/2) = \frac{1}{2}\coth(K/2)$. This result has previously been obtained by Kadanoff.[21]

The Potts models are more subtle. At first sight it appears that the thermal exponent y_T^P obtained from Eq. (7) is $2 - (2\theta_0)^{-1}$; but this is clearly incorrect since it gives $\alpha = \frac{1}{2}$ for the Ising model ($q = 2$). The resolution of this difficulty resides in the relationship among the coefficients D_i, peculiar to the Potts models (see Table I), which leads to a cancellation of the leading singularities in the free energy. The true thermal eigenvalue is given by what would normally be the leading correction to scaling, and this is proportional to the umklapp scattering variable y. A physical picture may be given in terms of the Coulomb-gas representation described above. The charges $\pm 2Q$ associated with y are twice as large as those associated with $D^{\pm}$ [$(2\theta)^{-1} \rightarrow 2/\theta$ in going from Eq. (7) to Eq. (5) so $Q^2 \rightarrow 4Q^2$]. The Potts-model cancellation means that, asymptotically, there are no bare charges of value $+Q$ (fugacity D^+), and the insulating phase cannot consist of bound pairs of charge $\pm Q$, but rather the single charges disappear into bound triplets ($-Q, -Q, 2Q$). Consequently $2y_P^T$ is the dimension of $(D^-)^2 y$, and from Eqs. (5) and (7)

$$y_P^T = 3 - 3/2\theta_0 \tag{11}$$

a result which has been conjectured by den Nijs[1] on the basis of numerical values of y_T^P.

For $q = 0$, the cancellation can be seen directly from Table I and Eq. (4) ($\overline{D}_i = D_i/s$ and the bare value of $D^+ = 0$). For $q \neq 0$, we have established it analytically to first order in g and numerically for all g in the range $0 \leq g < 1$ by means of the matching procedure described above. The latter provides a boundary condition for Eq. (7), leading to the solution

$$D^+(l) = D^-(l) \tanh I(l) \ , \tag{12}$$

$$D^-(l) = \frac{\cosh I(l)}{\cosh I(l_i)} D^-(l_i) \exp[K(l)] \ , \tag{13}$$

where

$$I(l) = \frac{1}{2} \int_l^\infty dl' \, y(l') \ ,$$

$$K(l) = \int_{l_i}^l dl' \, [2 - (2\theta)^{-1}] \ ,$$

and l_i is the matching point. For $\theta_0 < 1$,

$$I(l) \sim y(l) \exp[(2 - 2/\theta_0) l] \rightarrow 0$$

asymptotically so Eq. (12) gives $D^+(l) \sim D^-(l) I(l)$. In the same region $K(l) \sim l[2 - (2\theta_0)^{-1}]$ and, since $df/dl \sim D^+D^-$, Eq. (11) follows immediately from the usual procedure for determining thermal exponents. On the other hand, when $\theta_0 \geq 1$, or $q \geq 4$, the integral defining $I(l)$ diverges at its upper limit and, according to Eq. (12), $D^+(l) = D^-(l)$ and there is no further cancellation.

The four-state Potts model is of special interest. This is the point ($g=1$) for which the trajectories flow into $\theta=1$, $y=0$. Setting $2-2/\theta \equiv -x$, the solution of Eqs. (5) and (6) near the fixed point is given by $x=y=(a+l)^{-1}$ and, since $2-(2\theta)^{-1} \simeq \frac{3}{2}-x/4$, we obtain Nauenberg and Scalapino's result[22] for the free energy: $f \sim t^{4/3}/|\ln t|$. This conclusion is identical to that obtained by Kadanoff[20] at the equivalent point of the Ashkin-Teller model, as it should be. For a finite-size system, a similar argument shows that $f \sim t^2 M(a+\ln M)^{-b}$ with $b=\frac{3}{2}$. Our numerical results are consistent with this form, with b in the range 1 to $\frac{3}{2}$. A similar logarithmic singularity is present in the free energy for all models; in particular it is present for weak dimerization in the ground state of spin-Peierls systems.[23]

For $q>4$ finite coherence length (10) for $t=0$ implies that the system is not at a critical point. It may be shown directly from the sine-Gordon representation that, in this region $f \sim |t|\xi^{-1/2}$ with ξ given by Eq. (10). The system then undergoes a first-order transition with latent heat $\sim\xi^{-1/2}$, in agreement with Baxter.[24]

Our picture of the Potts models has some similarity to that of Nienhuis *et al.*[7] and of Nauenberg and Scalapino[22]; the behavior near $q=4$ is associated with the existence of a marginal variable. However, we do not have to introduce dilution for this purpose; the marginal variable is already present in the lattice model as umklapp scattering. We also emphasize that our derivation of renormalization-group *equations* (5)–(7) did not make use of any exact results or conjectures. The only external input is the global relation (9) which serves as a *boundary condition* on the solutions.

A discussion of electric and magnetic perturbations from this point of view will be given in a future publication, together with some considerations on tricritical exponents, and an expanded account of the work described in this communication.

After this work was completed, we received unpublished work from M. P. M. den Nijs, independently pointing out the role of umklapp scattering in the six-vertex model. Research was supported by the Division of Basic Energy Sciences, U.S. DOE, under Contract No. EY-76-C-02-0016.

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