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Exact Universal Amplitude Ratios in Two-Dimensional Systems near Criticality

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Universal amplitude relations associated with hyperscaling are obtained exactly for several integrable perturbations of two-dimensional (multi)critical points described by minimal models. The results are confirmed numerically and it is discussed how they can be verified by experiment.

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At a critical point, the long-distance behavior of a system is given by a scale-invariant continuum field theory. The simplest two-dimensional such theories are the series of minimal models M_m $(m=3,4,\ldots)$, whose first member M_3 is the critical Ising model. They can be classified and solved exactly by means of their infinite-dimensional conformal symmetry [1,2]. In heat capacity and scattering experiments, the leading exponents of these universality classes have been measured in a variety of systems [3]: Ising critical behavior was found in two-dimensional antiferromagnets such as K_2CoF_4 at the Néel point [4] and in the reconstruction transition of Au surfaces [5]; melting transitions of atomic submonolayers adsorbed on crystal surfaces fall into the Ising [6] or the three-state Potts universality class M_5 [7], or have continuously varying exponents, depending on the symmetries of the crystal surface and the microscopic interactions [8].

Perturbing the critical theory by a generic combination of its relevant scaling fields destroys all long-range correlations and generates a finite correlation length ξ, defined by the weakest exponential asymptotic behavior $\sim e^{-r/\xi}$ of the two-point functions. The resulting massive renormalized field theories describe the scaling region around the critical point, where the ξ is much larger than any microscopic length scale of the system. The correlation functions are determined entirely by those of the critical theory, but since the exponential decay is a nonperturbative effect, calculations are difficult in general. In two dimensions, however, important progress has been made recently for integrable perturbations (i.e., perturbations that retain an infinite-dimensional symmetry) of minimal models [9]. In several such cases, the exact S matrix of the associated one-dimensional quantum field theory has been conjectured. These scattering theories have a finite number of stable particles, and in all scattering processes the particle momenta are individually conserved. Numerically, the single-particle spectrum [10–13] and the elastic two-particle phase shifts [14,15] have been confirmed by transfer matrix diagonalization, but so far these conjectures lack any experimental verification. In this Letter, we point out that they lead to exact predictions of universal amplitude combinations [16] associated with hyperscaling relations [see Eqs. (2), (10), and (12) below]. This gives the first experimentally feasible test of the proposed scattering theories.

The finite-size scaling hypothesis in d dimensions can be stated as follows: The singular part of the free energy F (measured in units of k_BT) of a system with volume R^d is, on a given renormalization-group (RG) trajectory, a universal function of the dimensionless variable R/ξ only [17]. In particular, in the thermodynamic regime, where all linear dimensions of the system are $\gg\xi$, the most singular term is proportional to the volume:

$$F(R/\xi)=\epsilon_0(R/\xi)^d+\cdots\,, \tag{1}$$

where the bulk constant ϵ_0 is universal [18]. Corrections to this asymptotic behavior are less-singular universal terms that depend on the boundary conditions and the shape of the sample (such as a surface term $\sim\xi^{-(d-1)}$), and nonuniversal background terms that remain analytic in the thermodynamic limit. The latter contain powers of the microscopic lattice cutoff a and are subtracted in the renormalized continuum theory. For a RG trajectory whose points are parametrized by a single coupling constant λ with scaling dimension y, the finite-size scaling hypothesis implies *one-scale-factor universality*: The only system-dependent quantity for all variations of the free energy along this trajectory is the scale factor $g \equiv \lambda \xi^y$. The dimensionless combinations

$$\frac{\lambda \partial_\lambda F}{R^d} \xi^d = \frac{d}{y} \epsilon_0 + \cdots ,$$
$$\frac{\lambda^2 \partial_\lambda^2 F}{R^d} \xi^d = \frac{d}{y} \left(\frac{d}{y} - 1 \right) \epsilon_0 + \cdots , \ \ldots , \tag{2}$$

which involve the thermodynamic density conjugate to λ, the response function, etc., are independent of this scale factor and hence universal as well. Examples are discussed below.

Recall that the free energy of a two-dimensional classical system defined on a rectangle $R \times L$ with periodic boundary conditions equals that of a one-dimensional quantum system defined on a circle of perimeter R, at inverse temperature (imaginary time) L. The quantum Hamiltonian $H(R,\xi)$ is obtained by integrating the time-time component of the renormalized stress-energy tensor along this circle [19]. The important conclusion is that the free energy of this quantum system is precisely the *universal* free energy of the two-dimensional system near criticality. In the low-temperature limit $L \to \infty$, it behaves as $F \simeq L E_0(R,\xi)$, where $E_0(R,\xi)$ is the ground-state energy of the Hamiltonian $H_0(R,\xi)$. By quantizing the system in the perpendicular direction and thus exchanging the roles of space and imaginary time, one sees that $E_0(R,\xi)$ is also the grand canonical pressure of the system in the thermodynamic limit, at inverse temperature R.

For several integrable systems, this quantity has been obtained exactly by means of the thermodynamic Bethe ansatz (TBA) [20]. The basic idea is as follows. The pressure of such a system can be written in the same form as for a free quantum gas, $E_0 = \mp \sum_a \int (dk/2\pi) \times \ln(1 \pm e^{-\varepsilon_a(k)})$ (a labels different particle species); the effect of the interactions is contained in the Boltzmann weights $e^{-\varepsilon_a(k)}$. Particle momenta are conserved individually; hence the only effect of a scattering process on a particle is a phase shift between in and out wave functions. As these wave functions have to match when continued around the circle, the phase shift changes the energy of the level. In the thermodynamic limit, this amounts to a change in the spectral density which can be absorbed in the $\varepsilon_a(k)$. For the theories of interest here, the solution of the TBA equations yields in particular a simple expression for the bulk constant ϵ_0 in terms of the elastic S matrix of two lightest particles as a function of the Lorentz-invariant rapidity difference $\theta = \theta_1 - \theta_2$ [20,21],

$$\epsilon_0^{-1} = -\frac{2}{i} \lim_{\theta \to \infty} \left(e^\theta \frac{d}{d\theta} \ln S(\theta) \right) , \tag{3}$$

which in turn is determined completely by the poles θ_b of $S(\theta)$,

$$\epsilon_0^{-1} = -4 \sum_b \sinh\theta_b . \tag{4}$$

Actually, Eq. (3) has a very simple interpretation in terms of the scattering process shown in Fig. 1 in the c.m. frame. By taking Gaussian in and out wave packets,

$$\phi_1^{\text{in}}(t,r) = \int d\theta' e^{-(1/2)(\theta'-\theta_1)^2} e^{iE(\theta')t - ik(\theta')r} ,$$
$$\phi_1^{\text{out}}(t,r) = \int d\theta' e^{-(1/2)(\theta'-\theta_1)^2} S^{-1}(\theta'-\theta_2) e^{iE(\theta')t - ik(\theta')r} \tag{5}$$

(and in an analogous way for particle 2), we can show that the inverse bulk constant is actually the simple *classical* Lorentz invariant

$$\epsilon_0^{-1} = -\lim_{\theta \to \infty} (K \cdot X)(K \cdot K)/m_1^2 , \tag{6}$$

where K is the intermediate 2-momentum and X is the world vector characterizing the scattering process of Fig. 1. Hence it is proportional to the c.m.-frame time delay that either particle suffers as a result of scattering off the other. Remarkably enough, this very simple observable of the classical relativistic dynamics in one dimension corresponds to one of the most fundamental quantities of the universal thermodynamics in two dimensions.

Consider now the matrix elements of the quantum Hamiltonian $H(R,\xi)$ in a Hilbert-space basis that becomes an eigenbasis in the conformal limit $R/\xi \to 0$ [22]:

$$\langle i | H(R,\xi) | j \rangle = (2\pi/R)[-c/12 + x_i \delta_{ij} + (2\pi)^{1-y} g_0 (R/\xi)^y C_{i\Phi j}] , \tag{7}$$

where c is the central charge of the conformal theory, x_i are the dimensions, and $C_{i\Phi j} \equiv C_{\Phi_i \Phi \Phi_j}$ the structure constants of the (renormalized) scaling operators Φ_i (which are in one-to-one correspondence with the states $|i\rangle$). The primary [1] operators are normalized by the condition $\langle \Phi_i(0) \Phi_j(r) \rangle (\lambda = 0) = \delta_{ij} r^{-2x_i}$ on their two-point

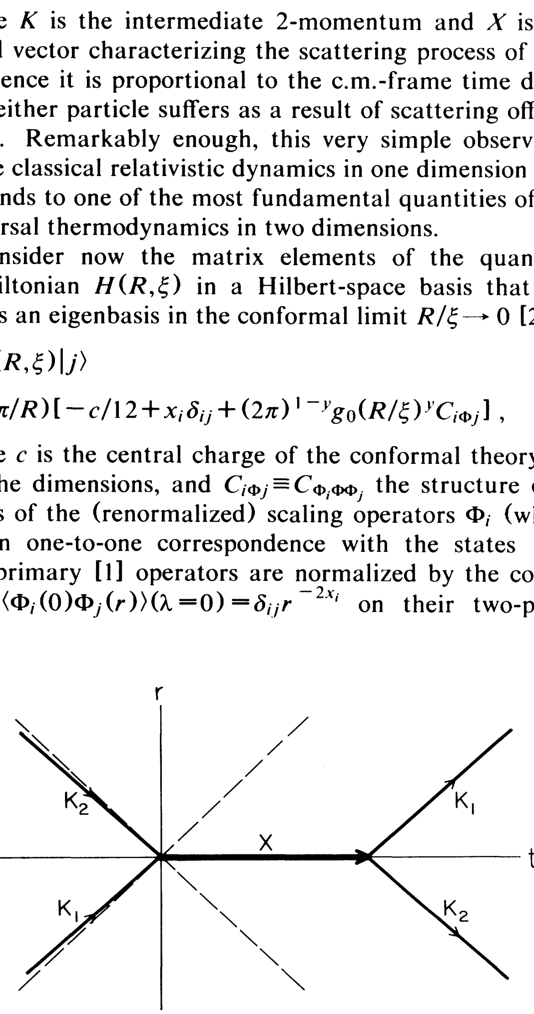

FIG. 1. Minkowski diagram describing the elastic scattering of two ultrarelativistic particles of mass m_1 in the c.m. frame. The process is characterized by the intermediate momentum $K = K_1 + K_2$ and the timelike vector X measuring the space-time delay between ingoing and outgoing particles.

functions in the plane. This choice now fixes the scale factor, which appears as the dimensionless coupling constant $g_0 = \lambda_0 \xi^y$ in (7). Below, we shall identify g_0 with another important universal amplitude combination on the RG trajectory parametrized by λ. By comparing the solution of the TBA equations in the high-temperature limit $R \to 0$ with conformal perturbation theory, this constant can be obtained exactly as well [20]. For the experimentally relevant cases, namely, the magnetic perturbation of the Ising model [9], and the leading thermal perturbation of the tricritical Ising model M_4 [23] and the three-state Potts model [24], the values of ϵ_0 and g_0 are collected in Table I.

The results of the TBA can be verified with great accuracy by the conformal truncation method [12,13]. This *nonperturbative* approximation consists in restricting the Hilbert space to the finite-dimensional subspace spanned by the states $|i\rangle$ with $x_i < x_{\max}$. The low-lying spectrum of H can then be obtained by diagonalizing a finite-dimensional matrix. For $x_{\max} \gtrsim 3$, the vacuum energy density E_0/R becomes independent of this cutoff and for $R > \xi$ converges rapidly to its bulk value ϵ_0, whose best numerical estimates are presented in Table I. The data for the (presumably not integrable [13]) leading magnetic perturbation of the tricritical Ising model are included as well [25]. The single-particle spectrum below the threshold of this theory (measured in units of the lightest mass m_1) equals that of the Ising model in a magnetic field to about 1% [11,13]. Interestingly, the bulk constants differ drastically and Eq. (4) is not even approximately correct for this model, which makes the similarity of the mass spectra appear even more surprising.

How could one measure universal amplitudes like (1) in practice? For definiteness, consider an Ising (anti)ferromagnet in a (staggered) magnetic field, although analogous arguments apply to the other cases of possible experimental interest, namely, dilute antiferromagnets or metamagnets at a tricritical point, or adsorbed Potts lattice gases [26]. The connected order-parameter correlation functions in momentum space, which are accessible

TABLE I. The bulk constant ϵ_0, the dimensionless coupling constant g_0, and the universal constant Δ_0 for several perturbations of minimal models. For ϵ_0 and g_0, the first value is taken from the TBA results of Refs. [20,21]; the second value is obtained by conformal truncation.

Model, perturbation	ϵ_0	g_0	Δ_0
Critical Ising,	-0.06173	0.06203	2.397×10^4
magnetic	$-0.0617 \pm 0.1\%$	...	
Tricritical Ising,	...	...	4.31×10^4
magnetic	$-0.140 \pm 0.5\%$	0.103	
Tricritical Ising,	-0.09421	0.09283	3.985×10^3
thermal	$-0.094 \pm 0.5\%$	...	
3-state Potts,	-0.02887	0.16430	7.490×10^2
thermal	...	...	

in a scattering experiment, can be written in scaling form,

$$G(q,\lambda) = \chi(\lambda) D(\kappa) , \tag{8}$$

where $G(0,\lambda) \equiv \chi(\lambda) = -\partial_\lambda^2 F/R^2$ is the susceptibility divided by $k_B T_c$ and $\kappa \equiv |q|\xi$. In order to obtain ξ, one would usually fit the data with a Lorentzian $D(\kappa) = (1+\kappa^2)^{-1}$, assuming that this function is dominated by single-particle poles at $\kappa = \pm i$. Here, however, its analytic structure is much more complicated: There are 2×8 single-particle poles and many branch cuts [27] of two and more particles. This makes it impossible to extract the "true" real-space correlation length ξ directly from the momentum space measurements. The length scale $\tilde{\xi} \equiv [-\frac{1}{2}\partial_\kappa^2 D(\kappa)|_{\kappa=0}]^{1/2}\xi$ defined by the infrared behavior of $D(\kappa)$ corresponds to the second moment of the real-space correlations and is universally related to ξ. The bulk amplitude equivalent to (1) has been obtained [28] from the c theorem [29]:

$$\frac{F}{R^2}\tilde{\xi}^2 = -\frac{1}{36\pi}\frac{c}{2-y} + \cdots . \tag{9}$$

Comparing this with (1) and (4) yields the universal ratio $\xi/\tilde{\xi}$ ($=1.3211$ in this case), which measures the contribution of the higher singularities to $D(\kappa)$, i.e., the deviation of its shape from a Lorentzian. Without further assumptions on this shape, the scale $\tilde{\xi}$ is difficult to extract from the scattering data as well, due to their error margins for wave numbers $q \ll \xi^{-1}$.

Alternatively, one may relate ξ to the universal ultraviolet asymptotics of $G(q,\lambda)$, which can be observed for wave numbers $\xi^{-1} \ll q \ll a^{-1}$. This function has to remain finite as $\xi \to \infty$, and hence $D(\kappa)$ behaves as κ^{d-2y} in this limit. Substituting this and (2) into (8), one concludes that

$$\lambda^2 \left[\lim_{q\to\infty} G(q,\lambda) q^{-d+2y}\right] \xi^{2y} = a_0 g_0^2 \tag{10}$$

is a finite universal number. In conformal field theory, the normalization condition is $G(r,\lambda) \simeq r^{-2(d-y)}$ in real space and hence $G(q,\lambda) \simeq a_0 q^{d-2y}$; this defines the numerical constant a_0 $[=2^{2(y-1)}\pi\Gamma(y-1)/\Gamma(2-y)$ for $d=2]$. Evaluating the left-hand side of (10) in this normalization then shows that g_0 equals the known dimensionless coupling constant that appears in (7).

If we combine (2) and (10) to eliminate the inaccessible quantity ξ, we get a prediction for a *feasible* experiment, which is the central result of this Letter: The universal amplitude

$$\Delta_0 \equiv a_0^d g_0^{2d} [(d/y)(d/y-1)\epsilon_0]^{-2y} \tag{11}$$

(which is evaluated in the last column of Table I for the cases of interest) is completely determined by the scattering data at $q=0$ and in the ultraviolet tail,

$$\lambda^{2d-4y} \left[\lim_{q\to\infty} G(q,\lambda) q^{-d+2y}\right]^d \Big/ G(0,\lambda)^{2y} = \Delta_0 . \tag{12}$$

The amplitude in the numerator can be determined more accurately if corrections to the leading ultraviolet behavior are taken into account. Powerlike corrections are of the form [30] $D(\kappa)\sim\kappa^{d-2y}\sum_i\sum_{n=0}^{\infty}A_{i,n}\kappa^{-x_i-ny}$. The universal correction-to-scaling amplitudes $A_{i,n}$ are of considerable interest in their own right since they provide a way of measuring the operator product algebra of the conformal theory. They can also be evaluated accurately by conformal truncation. Many of them vanish by symmetry. Specifically, for the Ising model in a magnetic field, one obtains the expansion $D(\kappa)\sim\kappa^{-7/4}[1+A_{2,0}\kappa^{-1}+A_{1,1}\kappa^{-2}+O(\kappa^{-15/4})]$, taking into account the leading contributions of the lowest three scaling operators, which have dimensions $x_0=0$, $x_1=\frac{1}{8}$, and $x_2=1$. In fact, it is possible to combine this information with Eqs. (1), (4), (9), and (10) to construct an approximation to the whole scaling function $D(\kappa)$. This will be the subject of a future publication.

In summary, we have shown how the bulk constant ϵ_0 and the dimensionless coupling constant g_0, which are known exactly in integrable theories, are related to surface scattering experiments. These numbers depend on detailed predictions of conformal field theory, S-matrix theory, and the bootstrap principle at a nonperturbative level. Such an experiment could test these fundamental ideas.

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