

Criticality in One Dimension with Inverse Square-Law Potentials

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We demonstrate that the scaled order parameter for ferromagnetic Ising and three-state Potts chains with inverse square interactions exhibits a *universal* critical jump, in analogy with the superfluid density in helium films. Renormalization-group arguments are combined with numerical simulations of systems containing up to 10^6 lattice sites to accurately determine the critical properties of these models. In strong contrast with earlier work, compelling quantitative evidence for the Kosterlitz-Thouless-like character of the phase transition is provided.

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One-dimensional scalar models with inverse square potentials have held a special position in the field of statistical mechanics for several decades. The surprisingly rich behavior emerging from these conceptually simple systems has attracted the attention of a variety of workers in the field. The work of Ruelle [1] and Dyson [2] proved that pair interactions decaying as $1/r^2$ (where r denotes the distance between two local variables) represent the boundary between models with and without a phase transition at nonzero temperature; but it took until the 1980s before Fröhlich and Spencer [3] proved rigorously the existence of a phase transition for the borderline case itself. Meanwhile, early work by Anderson and Yuval [4] (who were motivated by the connection to the Kondo problem) had suggested that this phase transition has a special character, with an order parameter that exhibits both a discontinuity *and* a superposed singularity at the critical point. This behavior later gained widespread attention through the Kosterlitz-Thouless (KT) transition in the two-dimensional (2D) XY model [5]. Indeed, the vortex-unbinding scenario in the latter case has a direct analog in terms of logarithmically interacting defects (domain walls) in the “kink-gas” representation of the Ising chain considered in [4]. This treatment in the spirit of the renormalization-group (RG) theory was extended in [6] and most notably by Cardy [7], who demonstrated that it can be generalized to large classes of discrete models. In this sense, these one-dimensional models can be considered as the simplest examples of the class of “topological” phase transitions, which comprises phenomena such as 2D superfluidity and superconductivity, as well as dislocation-mediated melting of crystals.

An exact lower bound on the critical order-parameter jump has been obtained by Aizenman *et al.* [8] for Ising and Potts chains with $1/r^2$ interactions, and the existence of an intermediate ordered phase, where the correlation function decays as a temperature-dependent power law, has been proven by Imbrie and Newman [9]. Despite these rigorous results the literature on these models contains various contradictory claims and unconfirmed conjectures, while few of the RG-based predictions for the critical properties

have been verified by alternative methods: Thus (i) the critical temperature T_c has been estimated by a great variety of techniques, but little consistency has been obtained until now, with estimates differing by up to 30%. Indeed, there is even a conjecture for T_c of the q -state Potts chain that is *independent* of q [10], despite the fact that this appears to contradict intuitive energy-entropy arguments. (ii) In contrast, it has been claimed on the basis of numerical simulations that the transition in the q -state Potts chain is continuous for $q \leq q_c$ and of first order for $q > q_c$ [11], although this in turn disagrees with the KT-like transition (with q -dependent exponents) found by Cardy [7]. (iii) It has been conjectured that the power-law exponent of the correlation function in the intermediate ordered phase is directly related to the value of the order parameter [9]. (iv) Numerical simulations have been unable to conclude whether the specific heat diverges at T_c or even whether it displays a maximum at T_c [12]. (v) No numerical work for a one-dimensional system has been able to reproduce one of the actual hallmarks of the KT universality class, namely, the predicted exponential divergence of the correlation length and the susceptibility for $T \searrow T_c$.

It is the aim of the present work to settle these open questions in a convincing way, although (ii) will be addressed only partially, by combining finite-size scaling relations obtained from the RG predictions (which until now have been ignored in nearly all numerical studies) with accurate numerical simulations that span an unprecedented range in system sizes. Indeed, the long-range nature of the interactions has posed a major hurdle for the numerical study of these models: Whereas almost two decades ago Monte Carlo (MC) simulations could reach a system of $L = 256$ lattice sites [12], the most recent work still could attain only $L = 900$ [11]. By using appropriate techniques, we have now been able to study systems as large as $L = 10^6$. This allows us not only to answer questions intrinsic to the one-dimensional systems under study, but also to obtain what we believe are the most accurate numerical results to date for a system exhibiting a KT-like phase transition: Indeed, although the 2D XY and Villain models have been examined in many numerical studies, it

has proven extremely difficult to obtain full consistency with the RG predictions [13]. Because of the exponential divergence of the correlation length ξ , it is essential to cover a large range in *linear* system sizes, which makes a one-dimensional system easier to study than a 2D one. In our analysis, we start from the hypothesis that the structure of the scaling functions is correctly described by RG theory, and examine the consistency between our numerical results and the scaling predictions to test the correctness of this hypothesis.

We have first focused attention on the Ising chain (or equivalently the $q = 2$ Potts chain), described by the reduced Hamiltonian $\beta\mathcal{H} = -K \sum_{\langle ij \rangle} s_i s_j / r_{ij}^2$, where the sum runs over all spin pairs, $s_i = \pm 1$, and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. We have carried out accurate MC simulations for chains of L lattice sites, with $10 \leq L \leq 10^6$, over a large temperature range. These results could be obtained owing to the use of a cluster algorithm that suppresses critical slowing down and has an efficiency that is *independent* of the interaction range [14].

Although the critical coupling K_c is a nonuniversal quantity, the large number of available estimates makes it interesting in its own right. In addition, its precise value proves indispensable if one wants to address the issues mentioned above. Since finite-size corrections decay only logarithmically near a KT transition, the determination of K_c is notoriously difficult, and a new approach has been found. To this end, we have relied on the observation that the properly scaled order parameter $\Psi \equiv K \langle m^2 \rangle$, with $m = L^{-1} \sum_{i=1}^L s_i$, is expected to exhibit a *universal* jump at the critical point. Indeed, as mentioned, it has been shown rigorously [8] that $\Psi(K > K_c) \geq \frac{1}{2}$ [whereas $\Psi(K < K_c) = 0$]. Furthermore, it was conjectured in [8] that this inequality is saturated at $K = K_c$ (which *seems* to be implied by the arguments of [4], but note the comments in [9]). While it can be easily shown that Ψ is invariant under a (real-space) RG transformation of the kink-gas representation of the Ising chain [15], it appears not to have been explicitly realized that the critical jump $\Psi_c \equiv \Psi(K_c)$ must be *universal*, in the sense that it will have the same magnitude in every system with couplings that decay *asymptotically* as r^{-2} . We remark that also for the analogous phenomenon in two dimensions (the celebrated universal jump in the superfluid density of a ^4He film) this universality was only realized [16] *after* the original work by Kosterlitz and Thouless [5]. In addition to the jump discontinuity, $\Psi(K > K_c)$ is predicted to exhibit a superposed singularity:

$$\Psi(K) = \Psi_c + a_1(K - K_c)^{\bar{\nu}} + a_2(K - K_c)^{2\bar{\nu}} + \dots, \quad (1)$$

with $\bar{\nu} = \frac{1}{2}$ for the Ising chain; the ellipsis also includes nonsingular correction terms. In what follows, we demonstrate how to exploit the scaling properties of Ψ to accurately locate K_c . Figure 1 shows $\Psi(K, L)$ as a function of K for different system sizes. While Ψ is already sharp-

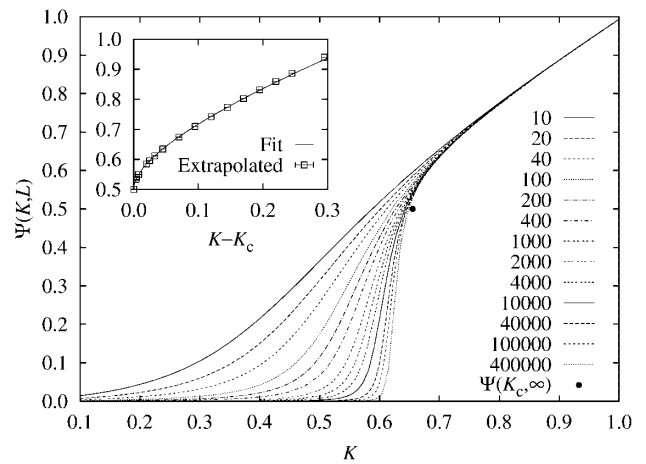


FIG. 1. The scaled order parameter $\Psi \equiv K \langle m^2 \rangle$ of the inverse square Ising chain, as a function of the coupling K . The inset shows the estimates for $\lim_{L \rightarrow \infty} \Psi(K, L)$ for $K > K_c$, along with a fit of the predicted singularity.

ening up for relatively small L , it is only for very large systems that one observes the development of a discontinuity and an additional singularity.

To proceed further, we recall the lowest-order RG flow equations [4,6] for the coupling and the defect fugacity y , namely,

$$dK/dl = -4Ky^2, \quad (2)$$

$$dy/dl = -y(2K - 1), \quad (3)$$

which (under the additional assumption that the system size scales with the rescaling parameter e^l) allow us to derive the finite-size scaling behavior of $\Psi(K, L)$ in the low-temperature regime. Since this derivation is somewhat involved [15], we only quote the final result here, namely,

$$\Psi(K, L) = \Psi(K, \infty) \times [1 + b_1 L^{-2(\bar{\Psi}-1)} + b_2 L^{-4(\bar{\Psi}-1)} + \dots], \quad (4)$$

where $\bar{\Psi} \equiv \Psi(K, \infty)/\Psi_c$. Nonsingular corrections become important only when $\Psi > 2\Psi_c$. The appearance of $\Psi(K, \infty)$ both as an amplitude and as an exponent is typical for a KT transition. A least-squares fit of this equation to $\Psi(K, L)$ has been used to obtain $\Psi(K, \infty)$ for several values of K , as shown in the inset of Fig. 1. This also yielded $\Psi_c = 0.49 \pm 0.02$. Keeping Ψ_c fixed at the predicted value $\frac{1}{2}$ [8,15] yielded $K_c = 0.6552$ (2). Subsequently, Eq. (1) allowed us to determine $\bar{\nu} = 0.52 \pm 0.03$. We have supplemented this low-temperature approach with an analysis of data lying within the high-temperature finite-size regime, where $L \ll \xi$ and $K < K_c$. The algebraic corrections in (4) now become powers of $1/\ln L$ and temperature-dependent terms take the form L/ξ , with $\xi = \exp[B/(K - K_c)^{\bar{\nu}}]$ [15]. We then find $\Psi_c = 0.496$ (3), in excellent agreement with the RG

prediction, and $K_c = 0.6548$ (14). Keeping Ψ_c now fixed at $\frac{1}{2}$ yields $K_c = 0.6555$ (4), very close to the value resulting from the low-temperature approach.

Independent estimates for K_c and $\tilde{\nu}$ can be obtained from the high-temperature susceptibility, which should display the same exponential divergence as the correlation length. RG considerations regarding higher-order contributions [17] suggest $\chi \sim \exp[B_0(K - K_c)^{-\tilde{\nu}} + B_2(K - K_c)^{\tilde{\nu}} + \mathcal{O}((K - K_c)^{2\tilde{\nu}})]$. Numerical results for $L = 4 \times 10^5$ and $L = 10^6$ are shown in Fig. 2, along with a truncated high-temperature expansion of order $\mathcal{O}(K^8)$ [18] and a fit to the RG expression. The agreement with the series expansion is good, but breaks down for $K \gtrsim 0.3$. The RG expression provides an excellent description of the MC data for $0.2 \leq K \leq 0.61$, confirming the predicted exponential divergence over a large temperature range. Owing to the covariance of the fit parameters, it is difficult to determine them simultaneously: We obtained $\tilde{\nu} = 0.54 \pm 0.03$ as our best estimate. However, keeping $\tilde{\nu} = \frac{1}{2}$ leads to $K_c = 0.6551$ (6), which we view as a strong confirmation of our analysis of Ψ . The rounding of χ close to K_c (see Fig. 2) is due to the finite system size. We estimate that the correlation length ξ is $\gtrsim 10^5$ here, which may be compared with a maximum of $\xi \approx 140$ reached in recent $d = 2$ simulations [13].

Subsequently, we carried out a similar analysis of Ψ and χ for the q -state Potts model with $q = 3$, which has a Hamiltonian of the form $\beta \mathcal{H}^{\text{Potts}} = -K^{\text{Potts}} \sum_{\langle ij \rangle} \delta_{s_i s_j} / r_{ij}^2$, with $s_i = 1, \dots, q$. Cardy [7] has found that, for positive integer q , this system can be described by RG equations that are very similar to those for the $q = 2$ (Ising) case, but yielding $\tilde{\nu} = 2/(q + 2)$. This implies that the entire analysis of the critical behavior can be carried through as before [15]: Ψ should still exhibit a universal jump (of magnitude 1 in units of K^{Potts}) with a superposed singularity as in (1) and χ

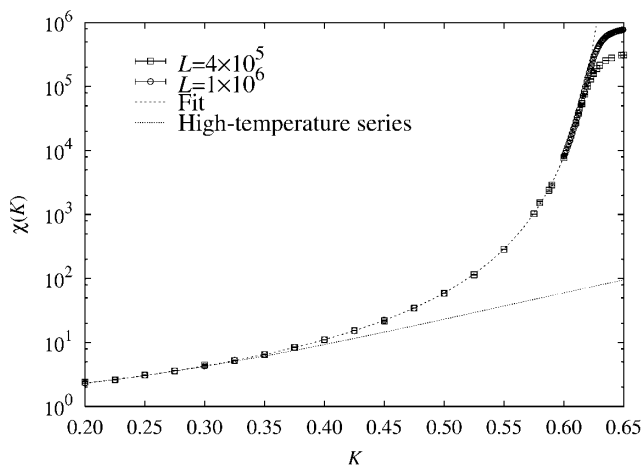


FIG. 2. The reduced magnetic susceptibility $\chi = L^d \langle m^2 \rangle$ of the inverse-square Ising chain as a function of the coupling, along with a (truncated) high-temperature series expansion [18] and a fit to the predicted asymptotic behavior $\exp[B_0(K - K_c)^{-\tilde{\nu}} + B_2(K - K_c)^{\tilde{\nu}}]$.

should again display an exponential singularity. The order parameter used for the determination of Ψ and χ is given by $m^{\text{Potts}} \equiv \max_{\alpha=1, \dots, q} [\frac{q}{L} \sum_{i=1}^L (\delta_{s_i \alpha} - 1)] / (q - 1)$, with $q > 1$. An analysis of Ψ for system sizes up to $L = 10^6$ yielded $K_c = 1.4105$ (2), $\Psi_c = 1.02$ (2), and $\tilde{\nu}(q = 3) = 0.41$ (2). A least-squares fit of the data for χ was consistent with an exponential divergence with $\tilde{\nu}(q = 3) = 0.42$ (2). Not only is Ψ_c in good agreement with the predicted universal value, but to our knowledge this is also the very first independent corroboration of the generalized RG scenario of Ref. [7], which predicts that $\tilde{\nu}(q = 3) = \frac{2}{5}$. As expected from entropic considerations, $K_c^{\text{Potts}}(q = 3)$ is somewhat higher than $K_c^{\text{Potts}}(q = 2) = 1.3104$ (4), which in turn refutes two conjectures based on a different real-space RG analysis [10], namely, that (i) K_c^{Potts} would be independent of q and (ii) K_c^{Potts} would be exactly given by $12/\pi^2 = 1.21585 \dots$. We note that our results are in strong contrast with earlier numerical work: Both a transfer-matrix study and a very recent MC study for $q = 2$ [19] and $q = 3$ [11,19] concluded that the correlation length diverges algebraically (rather than exponentially) with a q -dependent power-law exponent.

We now return to some interesting aspects of the Ising chain. First, it has been concluded in Ref. [12] that the critical spin-spin correlation function should decay logarithmically, $g(r) = \langle s_0 s_r \rangle - \langle s_0 \rangle^2 \sim 1/\ln r$, where now $\langle s_0 \rangle \neq 0$, unlike the situation for a typical critical phase transition. As illustrated in Fig. 3, we have been able to corroborate this behavior over a considerable range in r . In the high-temperature phase, the decay of $g(r)$ is bounded by the spin-spin interaction, but for $K > K_c$ it is expected that $g(r) \sim r^{-\theta}$, with $\theta = 4\sqrt{(K - K_c)/K_c}$ [12]. We note that this behavior would be consistent with the conjecture of Ref. [9], viz. that $\theta = \min[4(\Psi - \frac{1}{2}), 2]$ for $K > K_c$. We have determined θ for a large number of couplings, see Fig. 4,

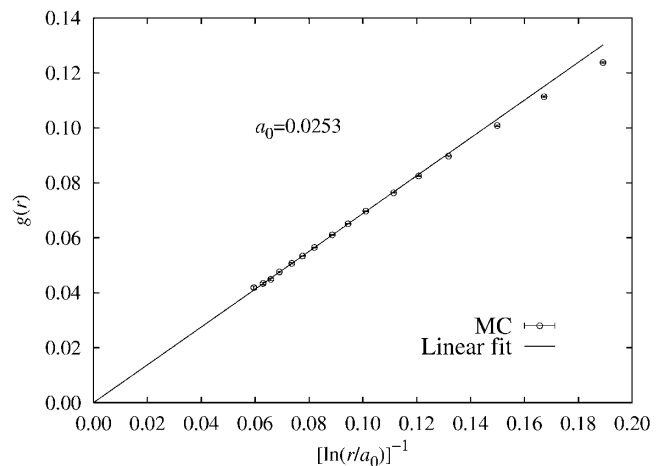


FIG. 3. The critical correlation function $g(r)$ of the inverse square Ising chain, for $5 \leq r \leq 5 \times 10^5$. The logarithmic decay can be followed for at least three decades in r .

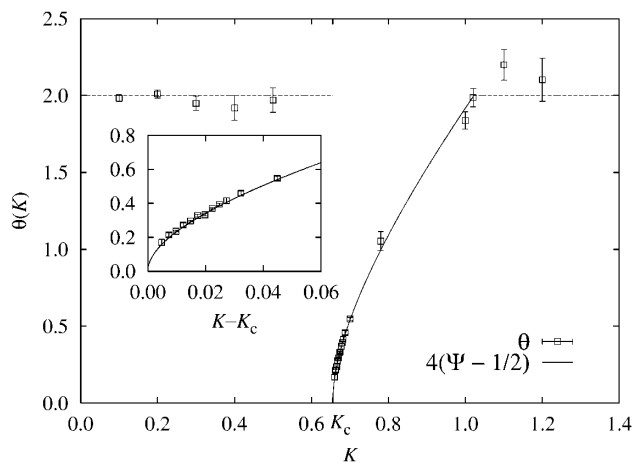


FIG. 4. The decay exponent θ of the spin-spin correlation function $g(r)$ of the inverse square Ising chain, as a function of the coupling. The inset shows an enlarged view of the region just below the critical temperature.

and have subsequently fitted these to a power series in $\sqrt{K - K_c}$, finding $\theta = (1.81 \pm 0.06)\sqrt{(K - K_c)/K_c}$. This agrees with $4a_1\sqrt{K_c} = 1.73(4)$, where a_1 is defined via Eq. (1), corroborating the conjectured relation with Ψ . However, the prefactor is approximately half as large as predicted in Ref. [12]. Farther away from K_c it becomes increasingly difficult to obtain accurate results for $\theta(K)$, owing to the rapid decay of $g(r)$. However, since our results corroborate the presumed relation between θ and Ψ , we exploit this relation to determine two special values of K , namely, the coupling strength K_1 for which $\theta = 1$ and the smallest coupling $K_2 > K_c$ for which $\theta = 2$. K_1 has the special property that the magnetic susceptibility will diverge over the full coupling range $K_c \leq K \leq K_1$, as follows from the fluctuation-dissipation theorem (and as is actually confirmed by the numerical results [15]). We find $K_1 = 0.78(1)$ and $K_2 = 1.02(3)$. Thus, the RG prediction $K_1 = \frac{17}{16}K_c \approx 0.696$ [12] is too low, due to the difference in the prefactor for $\theta(K)$. K_2 marks the end of the regime where $g(r)$ displays a leading temperature-dependent exponent.

Finally, we consider the specific heat C , which is calculated from the fluctuations in the internal energy. The efficiency of the original MC algorithm [14] is greatly reduced when this energy has to be calculated (although recently this problem has largely been overcome [20]) and hence only much smaller systems could be accessed. Nevertheless, this turns out not to be a limiting factor, since C has already converged within the range of accessible system sizes ($L \leq 16384$). We find unambiguously that C is a *nondivergent* quantity which takes its maximum at a temperature that lies approximately 14% above the critical temperature.

In summary, we have provided compelling evidence that the inverse square Ising and $q = 3$ Potts chain display

the one-dimensional analog of a Kosterlitz-Thouless transition, in disagreement with earlier numerical studies, but in accurate quantitative agreement with renormalization-group predictions. The (exponentially diverging) correlation length could be examined over more than 5 orders of magnitude, making this the most tractable KT-like transition.

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